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Chemotaxonomic Inference Under Metabolic Plasticity: Integrating Phylogeny, Tissue Specificity, Environment, and Specialized-Metabolite Profiles Without Treating Chemistry as a Fixed Species Trait

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ABSTRACT

Specialized-metabolite profiles are widely used to compare plant taxa, support identification, and interpret evolutionary differentiation, yet the chemical profile measured from a specimen is not necessarily a fixed expression of species identity. It is an observation produced jointly by inherited metabolic capacity, tissue and cell specialization, developmental and inducible state, environmental exposure, sampling time, and the analytical workflow used to recover and annotate chemistry. This article develops an original theoretical model for chemotaxonomic inference under such metabolic plasticity. The model separates independent phylogenetic evidence from biological chemical state and from the analytically observed metabolite representation, thereby preventing chemical similarity from being interpreted automatically as common ancestry or chemical difference as taxonomic separation. It further proposes that chemical traits should be interpreted according to whether their taxonomic information is stable across relevant contexts, conditional on explicitly matched contexts, or potentially misleading because biological or analytical states are mismatched. The framework retains convergence, rapid lineage divergence, inducible metabolism, seasonal change, tissue compartmentation, and incomplete chemical identification as competing explanations rather than treating them as residual noise. For classification and authentication, the model favors concordance among chemistry, independent identity evidence, provenance, and context while treating discordance as an object of investigation. The framework is theoretical rather than prospectively validated; it supplies no universal marker thresholds, weighting coefficients, or diagnostic performance claims. Its principal value is to make the conditions under which chemical evidence can legitimately support taxonomic inference explicit and experimentally testable.

Keywords: Chemotaxonomy, Specialized metabolism, Metabolic plasticity, Metabolomics, Phylogeny, Botanical authentication

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Introduction

Plant specialized metabolites can carry substantial taxonomic information, but a useful chemical difference is not necessarily an immutable species character. Comparative metabolomic work in the *Ocotea* complex illustrates the problem directly: apparent chemophenetic separation can vary with the plant part examined and with the multivariate specification used to represent the chemical data [1]. The inferential difficulty is therefore not whether chemistry can distinguish plant material. It often can. The more demanding question is what a measured chemical pattern is evidence of: common ancestry, lineage-specific metabolic capacity, tissue composition, physiological state, ecological exposure, or the particular analytical window through which the sample was observed.

Ecology adds a second source of ambiguity. Secondary-metabolite distributions may be associated not only with lineage but also with processes structuring plant communities at regional and local scales [2]. Chemical resemblance among plants can therefore arise in contexts where ecological filtering, interaction history, or shared environmental demands contribute to the phenotype being compared. Conversely, close relatives need not exhibit identical realized chemistry when ecological conditions, organs, developmental states, or regulatory responses differ. Treating every metabolomic difference as taxonomic divergence risks converting a biologically responsive phenotype into an overly rigid species descriptor.

Integrative taxonomy offers a more appropriate epistemic precedent. When untargeted metabolomics is considered together with DNA-marker evidence and phenotype imaging, the chemical profile functions as one complementary information stream rather than as an unquestioned surrogate for identity [3]. This distinction is central to the theoretical model developed here. The article does not argue that specialized metabolites lack phylogenetic information or that chemical characters should be abandoned. Instead, it proposes that their inferential meaning must be conditioned on the biological and analytical circumstances under which they are expressed and measured.

Accordingly, the article distinguishes three objects that are often collapsed in chemotaxonomic reasoning: the lineage or taxonomic proposition under evaluation; the biological chemical state produced by inherited capacity interacting with tissue, development, signaling, and environment; and the observed chemical representation produced after sampling, extraction, ionization, feature detection, and annotation. These objects can coincide sufficiently for a chemical trait to be highly informative, but their correspondence should be demonstrated rather than assumed. The proposed model therefore treats chemotaxonomic inference as a problem of contextualized evidence integration. It asks when a chemical signal remains stable across relevant contexts, when it is conditionally informative only under matched contexts, and when apparent taxonomic information may instead reflect biological plasticity or measurement structure. This formulation preserves the evolutionary value of phytochemistry while making its uncertainty explicit.

The changing meaning of a chemotaxonomic signal

A chemotaxonomic signal begins as biological chemistry but reaches the analyst only through an observation process. In untargeted analysis of Malpighiaceae, extraction strategy and ionization conditions altered which regions of specialized-metabolite space were recovered and compared [4]. Thus, absence from an analytical profile is not equivalent to biological absence, and relative prominence in a dataset is not automatically proportional to biological abundance. The operative taxonomic signal is partly constructed by sample preparation and instrumental detectability.

The evidential status of a detected entity also matters. Best-practice guidance for mass-spectrometry metabolomics distinguishes detected features, annotations, structural identifications, and quantitative measurements rather than treating these as interchangeable levels of certainty [5]. Chemotaxonomic interpretation should preserve the same distinction. A reproducible but unidentified feature may support discrimination among samples; an assigned molecular formula, predicted chemical class, library match, and experimentally confirmed structure support progressively different claims. None of these levels, by itself, establishes taxonomic specificity.

Modern computational workflows increase interpretable coverage without eliminating this boundary. Feature-based molecular networking can organize chromatographically resolved features according to fragmentation similarity while retaining quantitative and sample metadata [6]. Such relationships are valuable for exposing coordinated chemical families, but network adjacency does not prove that two features are identical structures or that a network cluster corresponds to a clade. Likewise, computational classification of high-resolution fragmentation spectra can assign chemical classes to metabolites that remain structurally unresolved [7]. Class-level coverage can therefore reveal broad patterns missed by compound-by-compound identification, while still remaining distinct from exact structural proof.

The meaning of “chemical character” consequently changes with analytical resolution. At one extreme it may denote a verified metabolite structure; at another it may denote a reproducible spectral feature or a predicted chemical family. The proposed model treats this hierarchy as an analytical-confidence boundary: taxonomic interpretation should not silently exceed what the underlying chemical assignment supports. A chemical pattern can remain useful below full structural identification, but its inferential claim must be stated at the same evidential level. Chemotaxonomy under modern metabolomics is therefore not simply a larger version of classical marker

chemistry. It is an inference problem in which measurement, annotation, and biological interpretation must remain separable.

Phylogenetic and biological sources of chemical pattern

The first requirement for interpreting chemistry as evolutionary evidence is an independent representation of lineage relationships. Large-scale plant phylogenomics demonstrates that evolutionary structure can be reconstructed from extensive sequence information independently of metabolite profiles [8]. Such a scaffold allows chemistry to be tested against phylogeny rather than being used simultaneously to define and confirm the same relationships.

Specialized metabolism can nevertheless contain genuine evolutionary signal. Integrative reconstruction of a plant-defense pathway has shown how changes in genes and enzyme functions can generate biochemical innovation through evolutionary time [9]. At the level of phytochemical characters, however, explicit mapping onto phylogeny can reveal gains, losses, and homoplasy rather than simple inheritance of fixed compounds, as illustrated in *Pilocarpus* [10]. Chemical characters therefore record evolutionary history imperfectly: they can reflect descent while remaining capable of repeated loss, innovation, or reappearance.

The same tension is visible in broader metabolomic comparisons. Evolutionary metabolomics across *Nicotiana* identified lineage-associated innovations while also exposing substantial diversification within the genus [11]. In *Inga*, secondary metabolism likewise exhibited phylogenetic structure together with pronounced divergence among related lineages [12]. These findings make phylogenetic scale important. A chemical pattern may be informative at one taxonomic depth and unstable at another, particularly when recently evolving pathways or regulatory states dominate the measured profile.

A second complication is non-unique evolutionary origin. Plant specialized metabolism is highly evolvable, and similar metabolic outcomes may arise through pathway reuse, co-option, or convergence [13]. Species-specific or lineage-restricted genomic regions can also contribute to metabolic polymorphism, but genomic capacity does not imply constitutive expression of the corresponding chemistry in every organ or environment [14]. Consequently, chemical similarity may represent common descent, deep biochemical conservation, convergent innovation, or shared regulation; chemistry alone cannot discriminate among these alternatives.

Biological compartmentation adds variation within a single organism. Asparagus roots and exudates show tissue-associated metabolite and protein signatures [15], while trichome-enriched metabolic machinery demonstrates that specialized metabolism can be concentrated at still finer cellular scales [16]. A leaf, root, exudate, epidermal structure, or reproductive organ is therefore not merely a different container for a fixed species metabolome. Sampling different biological compartments may interrogate different realized chemical states. The proposed framework accordingly treats tissue and cell context as explanatory variables that must be separated from lineage before a chemical difference is assigned taxonomic meaning.

Metabolic plasticity as a source of taxonomic uncertainty

Even when lineage and tissue are held conceptually separate, specialized metabolism remains dynamically responsive. Experimental analysis of plant defense has shown that metabolite diversity and organization can shift with defense-related state rather than behaving as static background composition [17]. Such plasticity is not necessarily random error. It can be biologically coordinated, yet still confound taxonomic inference when specimens are compared under unmatched physiological conditions.

Local signaling demonstrates how finely this conditionality can operate. During herbivory in *Nicotiana attenuata*, ethylene locally modulated jasmonate-dependent phenolamide accumulation [18]. A metabolite pattern measured from one position or perturbational state can therefore differ from another within the same plant even when genotype and nominal organ identity are unchanged. Taxonomic interpretation based on a single snapshot can inadvertently encode local signaling history.

Time is another independent dimension. Specialized-metabolite induction in *Brassica* crops follows temporally structured responses, making sampling time relative to perturbation consequential for the profile obtained [19]. Seasonal metabolomics in two Brazilian Cerrado species similarly identified season-associated shifts in multivariate chemistry [20]. Season should not be reduced to one causal variable: phenology, water availability, temperature, biotic exposure, and developmental progression may covary. Its importance for chemotaxonomy is that a reproducible seasonal profile can still be a conditional state rather than a constitutive species property.

Environmental similarity may also generate chemical resemblance across taxonomic boundaries. Comparative metabolomics of multiple Atacama plant species identified a shared set of metabolites associated with resilience in an extreme climatic setting [21]. Such commonality need not imply close ancestry; shared environmental pressure, conserved stress pathways, or both may contribute. More generally, induced specialized-metabolite states can differ with defense condition, local signaling, and perturbation timing [17-19]. The theoretical consequence is that environmental and physiological context should be modeled as a competing explanation for both chemical difference and chemical similarity.

Metabolic plasticity therefore changes the interpretation of variance. Instead of dividing observations simply into "taxonomic signal" and "noise," the proposed model distinguishes lineage-associated variation from context-associated biological variation and from analytical variation. These components can interact, and they may not be statistically separable in every dataset. The framework does not assume that plasticity weakens every chemotaxonomic marker. Rather, it asks whether the candidate signal persists across the contexts relevant to its intended use, changes in a predictable context-dependent manner, or becomes ambiguous when context is unknown. **Figure 1** summarizes this conditional architecture and shows how evidence-supported sources of chemical variation enter the proposed transition from observed profiles to taxonomic interpretation.

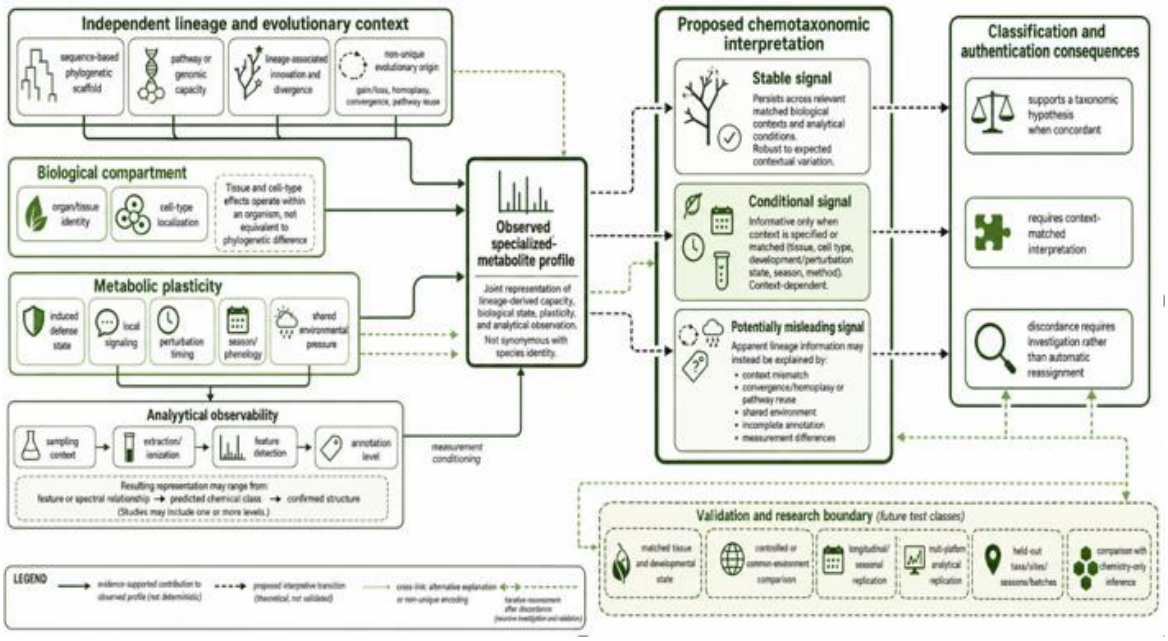

Figure 1. Conditional architecture of chemotaxonomic inference from lineage, biological state, and analytical observation

A revised model of chemotaxonomic inference

The preceding evidence suggests that a chemotaxonomic observation should be represented as the outcome of several partially independent processes rather than as a direct readout of species identity. Contemporary plant metabolomics expands chemical coverage, but interpretation remains conditioned by acquisition, annotation, and the functional meaning assigned to detected diversity [22]. The model proposed here therefore treats chemotaxonomic inference as a layered relation among an independent lineage hypothesis, a biologically realized chemical state, an analytically observed representation, and an interpretation made for a defined taxonomic purpose. The model is qualitative: it assigns no universal weights, thresholds, or confidence scores to these components.

The first distinction is between biological state and analytical representation. Extraction and ionization can change which portions of a metabolome are visible [4], so the observed profile should not be equated with the complete chemical state of the sampled organism. The second distinction is between chemical state and lineage. Sequence-based phylogeny provides an independent evolutionary scaffold against which chemical pattern can be interpreted [8]. This prevents circular reasoning in which chemistry simultaneously defines the groups and is then cited as

confirmation that the groups are chemically distinct. A chemically coherent cluster may support a lineage hypothesis, but only within the resolution and sampling conditions under which that coherence was demonstrated.
The third distinction concerns concordance and discordance among evidence streams. Integrative taxonomic analysis shows that metabolomics can contribute information complementary to DNA and phenotype data [3]. At the same time, similar metabolic outcomes can have non-unique evolutionary origins, including convergence or pathway reuse [13]. The proposed model therefore does not collapse discordant evidence into a single score. Instead, discordance is retained as information about possible context mismatch, analytical limitation, lineage complexity, or genuinely non-unique chemical evolution. Its interpretation should depend on which explanatory layer is inconsistent with the others.
This produces a simple decision principle: a chemical trait is most defensible as taxonomic evidence when the lineage hypothesis is independently defined, the biological compartment and state are relevant and comparable, the analytical representation is sufficiently characterized, and the observed chemical association persists across the contexts required by the intended inference. Where one or more conditions are not met, the evidence may still be useful, but the permitted claim narrows.
A further implication is that the unit of inference must be stated explicitly. “Species chemistry” is too coarse when evidence derives from one organ, population, season, developmental stage, or analytical platform. The relevant object may instead be a species-by-tissue profile, a lineage-associated chemical family, or a context-bounded distribution. Generalization is therefore treated as a transport problem: extension beyond the sampled context requires the biological and analytical assumptions supporting that extension to remain plausible.
The model also separates insufficiency from contradiction. Missing context narrows the permissible inference, whereas discordance between independently supported lineage and chemical evidence requires an explanatory account. **Table 1** organizes these components and the failure that follows when each is ignored.

Table 1. Proposed components of context-conditioned chemotaxonomic inference

Inferential component	Question asked	Permitted role	Failure if ignored
Independent lineage scaffold	What taxonomic relationship is being evaluated?	External evolutionary reference	Circular chemical classification
Biological chemical state	Which tissue, cell type, stage, or induced state was sampled?	Defines the realized phenotype	Context mistaken for lineage
Analytical representation	What chemistry was recoverable and at what annotation level?	Defines observable evidence	Non-observation mistaken for absence
Cross-context persistence	Does the association survive relevant matched contexts?	Supports broader inference	Conditional signal treated as fixed
Concordance or discordance	Do chemistry, identity evidence, and provenance agree?	Guides interpretation and follow-up	Conflict forced into a single verdict

Note. All components and decision roles in this table are proposed theoretical constructs; they are not validated diagnostic categories or quantitative confidence levels.

Stable, conditional, and misleading chemical traits

The usefulness of a chemical trait is not an intrinsic property of the molecule alone. Evolutionary ecology indicates that chemical-defense traits can differ in conservation and lability according to phylogenetic scale, ecological setting, and the trait considered [23]. The model therefore defines stability operationally: a stable chemotaxonomic signal is one whose association with the taxonomic proposition persists across the biological and analytical contexts relevant to its intended use. Stability is thus always stability *over specified conditions*, not an assertion that the compound is constitutively present in every specimen.
Comparative evidence also makes a binary stable-versus-unstable distinction inadequate. Lineage-associated innovation, rapid divergence among relatives, and convergently realized metabolic outcomes can coexist across specialized metabolism [11-13]. The proposed intermediate category is therefore a conditional signal: chemistry that is taxonomically informative when tissue, developmental or perturbational state, season, or analytical procedure is specified and matched. A conditional trait is not a weak trait by definition. For restricted questions, such as discrimination among consistently sampled organs under standardized analysis, it may be highly useful. The limitation is transfer: the inference should not silently extend beyond the conditions under which the association has been demonstrated.

A potentially misleading signal is different again. It is not a "bad molecule," but an observation whose apparent taxonomic meaning is vulnerable to an unresolved alternative explanation. Protocol-dependent recovery can create analytical mismatch [4]. Tissue-specific chemistry can create biological mismatch [15]. Seasonal shifts can create temporal mismatch [20]. Convergence, shared environmental responses, processing, or incomplete structural assignment can add further ambiguity. In such cases, stronger discrimination within a dataset may paradoxically coexist with weaker biological interpretation.

These proposed categories therefore classify the behavior of evidence rather than the essence of metabolites. A trait may move between categories as sampling expands or uncertainty is resolved. What appears stable in one tissue or site may become conditional after broader testing; what appears misleading may become informative once a confounder is explicitly controlled. Chemotaxonomic value is consequently a relation among trait, question, context, and evidence quality.

Importantly, "potentially misleading" is not synonymous with analytically erroneous. A measurement can be technically reproducible yet biologically misleading if the compared samples occupy different tissues, seasons, or induced states. Conversely, a conditional marker can be reliable when its conditions are deliberately standardized. The proposed classification therefore directs attention away from a search for universally invariant molecules and toward explicit statements of the domain over which a chemical association has been demonstrated. The broader the taxonomic or authentication claim, the more demanding the relevant domain of stability becomes.

Consequences for classification and authentication

Context-conditioned inference has practical consequences wherever chemical profiles are used to classify botanical material. Research-grade botanical studies benefit from explicit documentation of identity, provenance, cultivation or collection history, processing, and chemical characterization because these features can alter the material ultimately analyzed [24]. Within the proposed model, provenance is not an administrative supplement to chemistry. It is part of the evidence needed to decide whether a compositional difference is plausibly taxonomic, environmentally induced, processing-related, or simply the result of comparing non-equivalent materials.

Authentication poses a particularly useful test because it separates identity from composition. DNA barcoding and targeted metabolomic analysis of medicinal-plant samples can provide complementary information while remaining vulnerable to different limitations [25]. DNA evidence may be weakened by degradation, processing, mixed material, or marker resolution, whereas chemical evidence may vary with tissue, environment, extraction, storage, or substitution. Agreement between modalities can therefore strengthen interpretation, but disagreement should not automatically assign one modality as correct.

The model consequently proposes three authentication responses. First, concordant independent identity, provenance, and chemistry can support a taxonomic assignment within the validated scope of those data. Second, chemically discordant but independently identified material should trigger evaluation of tissue, state, environment, processing, or analytical method before substitution is inferred. Third, identity discordance accompanied by chemical discordance should prompt broader investigation rather than compression into a single similarity score. Authentication is therefore more defensible when chemical information is interpreted with independent identity evidence and documented provenance rather than treated as a sole species identifier [3, 24, 25].

This position does not diminish validated chemical markers. A marker may be entirely appropriate when its taxonomic specificity, relevant biological variability, analytical detectability, and material context have been established for the intended application. What the model rejects is automatic portability: a marker validated in one organ, developmental stage, geographic context, extraction method, or product type should not be assumed to retain the same inferential meaning elsewhere.

Classification and authentication also pose different inferential questions. Classification asks how chemical variation relates to taxonomic structure; authentication asks whether a particular material is consistent with a claimed identity under a defined product and sampling context. A chemically unusual authenticated specimen may therefore be informative about biological plasticity rather than evidence of misidentification, whereas a chemically typical sample does not independently establish identity. The same dataset can support different conclusions depending on which question is being asked and which external evidence constrains it.

The practical objective is not maximal multimodality for every sample, but evidence proportional to the uncertainty and consequence of the claim. In standardized applications, targeted chemistry may suffice; in processed, mixed, variable, or discordant material, stronger provenance and orthogonal identity evidence become more important.

Research questions generated by the model

The framework is useful only if its distinctions can be challenged empirically. A first question is how much observed chemical pattern remains attributable to lineage after biological compartment, physiological state, environment, and analytical procedure are varied. Plant-part sensitivity in chemophenetic analysis motivates matched-compartment comparisons [1]. Tissue-specific metabolite signatures further motivate designs in which organ or cell context is treated as a planned factor rather than uncontrolled heterogeneity [15]. Cross-species metabolomic commonalities under extreme environmental conditions likewise motivate common-garden or otherwise controlled environmental contrasts when the purpose is to distinguish lineage-associated chemistry from shared ecological response [21].

A second question concerns transferability. Context-aware inference should be compared with chemistry-only classification across held-out taxa, populations, sites, tissues, seasons, and analytical batches. Such evaluation should not ask merely whether a model discriminates the samples on which it was developed, but whether the inferred taxonomic relationship survives changes that the theory predicts should matter. Convergence is an especially demanding evolutionary hard case because similar chemistry may have non-unique origins [13]. Seasonality provides a temporal challenge in which a chemically discriminative pattern may shift even without taxonomic change [20]. DNA–chemistry discordance provides an authentication challenge in which alternative evidence streams can disagree for reasons that need explicit resolution [25].

A third question is whether the model's proposed evidence states are themselves useful. They could be tested by prospectively defining what constitutes a context expected to preserve a signal, then assessing whether traits classified as stable show greater cross-context persistence than traits classified as conditional. Likewise, deliberately mismatched tissue, season, or acquisition protocols could test whether predicted misleading states increase disagreement with independent identity evidence. Failure to observe these contrasts would weaken the proposed classification.

Finally, model evaluation should preserve the possibility of rejection. Appropriate studies would include factorial or common-garden designs, longitudinal sampling, replicated analytical platforms or ionization conditions, independent phylogenomic evidence, and prespecified hard cases. Ablation analyses could ask whether removing tissue, environment, time, or analytical-context variables changes out-of-sample interpretation.

Benchmark construction is itself consequential. Training and test sets drawn from the same tissue, location, season, and analytical batch may reward memorization of context-associated structure while appearing to support taxonomic generalization. More demanding evaluation would hold out one or more context dimensions deliberately and ask whether the same chemical interpretation survives. A useful benchmark should also retain discordant cases rather than removing them as inconvenient outliers, because those cases are precisely where the theoretical distinction between lineage signal and contextual chemistry is exposed.

No universal benchmark or acceptable performance threshold is proposed here. The central test is whether making context explicit yields interpretations that are more reproducible, transferable, and biologically coherent than treating the observed chemical profile as a fixed species trait. **Figure 2** converts these questions into a falsification-oriented validation architecture.

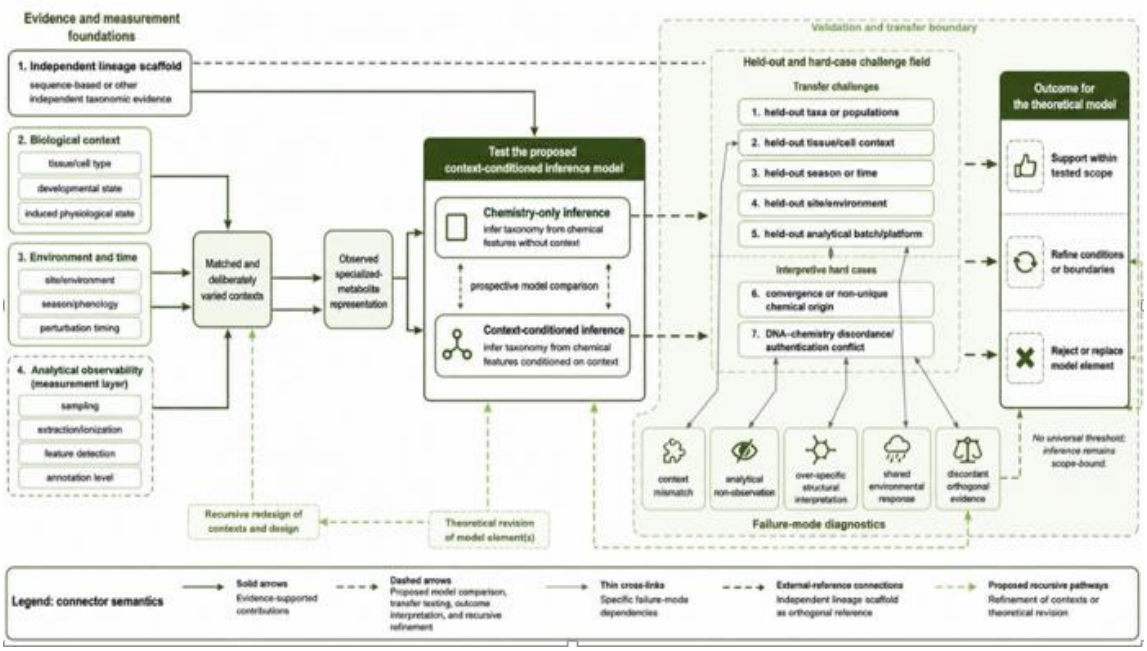

Figure 2. Falsification-oriented validation architecture for context-conditioned chemotaxonomic inference

Conclusion

Chemotaxonomic inference remains scientifically useful precisely because plant chemistry can contain evolutionary information, but that usefulness is weakened when the observed metabolite profile is treated as a fixed species essence. The theoretical model developed here separates lineage, biological chemical state, environmental and temporal plasticity, and analytical observability before asking what taxonomic claim a chemical pattern can support. Its central proposition is therefore conditional rather than anti-chemotaxonomic: chemistry should be interpreted according to the contexts across which its association with a taxonomic hypothesis is expected to persist.

The distinction among stable, conditional, and potentially misleading signals expresses this dependence without reducing it to a universal score. Stability requires relevant cross-context persistence; conditionality requires explicit specification of the context in which the signal is informative; and potentially misleading evidence requires active consideration of competing biological, evolutionary, or analytical explanations. For classification and authentication, concordance among chemistry, identity evidence, and provenance strengthens interpretation, while discordance should trigger investigation rather than automatic reassignment.

The model remains a theoretical synthesis. It does not establish universal marker classes, diagnostic thresholds, causal coefficients, or prospective gains in classification performance. Nor does it imply that every source of variation can be measured or partitioned. Interactions among lineage, environment, development, and analytical observability may remain inseparable, and some applications may lack sufficiently independent identity evidence. Its value will depend on whether matched-context experiments, longitudinal and environmental designs, multi-platform analysis, independent phylogenetic evidence, and out-of-sample hard cases support its distinctions. The strongest test is whether its contextual distinctions identify where chemical inference remains stable, where scope must narrow, and where discordance exposes an incorrect assumption. A chemotaxonomic framework able to survive those tests would not treat metabolic plasticity as nuisance variation to be erased. It would treat plasticity as part of the biological conditions under which chemical evidence acquires, retains, or loses taxonomic meaning.

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