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Chemical Identity Before Biological Activity: A Provenance-Centered Taxonomy for Separating Species, Plant Part, Extract, Fraction, and Isolated Natural-Product Evidence

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ABSTRACT

Natural-product research often treats botanical identity as though it were a single property that remains stable from a named species to the material placed in a biological assay. In practice, evidence may refer to a taxon, a defined plant part, a processed extract, a chromatographic fraction, an analytical feature, a candidate structure, or an isolated compound, and these objects are not evidentially interchangeable. This original classification article examines chemical identity as a provenance problem and proposes a taxonomy that separates material state from the confidence and scope of chemical identification. The synthesis distinguishes taxonomic/source identity, plant-part and material-form provenance, extract identity, fraction identity, and isolated-material identity, while treating chemical profiles, mass-spectrometric features, class assignments, candidate structures, and confirmed structures as separate analytical evidence states. A central principle is that biological evidence attaches first to the material actually tested; transfer to another pharmacognostic level requires an explicit bridge justified by shared provenance and appropriate analytical evidence. This prevents species names from functioning as proxies for extract composition, active fractions from being treated as proof of a single causal constituent, and computational annotations from being represented as established structures. The taxonomy is intended as an evidence-organizing framework rather than a validated scoring system or regulatory standard. Its usefulness will depend on reproducible classification, adequate reporting, orthogonal authentication where needed, and prospective testing of whether provenance-aware interpretation reduces unsupported evidence transfer.

Keywords: Pharmacognosy, Botanical authentication, Chemical provenance, Plant extracts, Fractionation, Natural-product structure

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Introduction

Natural-product pharmacology begins with a deceptively simple question: what, exactly, was tested? A biological result can be interpreted only in relation to a sufficiently defined experimental object. Best-practice guidance in phytopharmacology has emphasized that inadequately identified or characterized plant materials and extracts compromise reproducibility and weaken the interpretation of pharmacological findings [1]. Yet the conventional shorthand of a species name followed by an activity statement can conceal several transitions. The named organism may have supplied only one organ; that organ may have been dried, milled, extracted, partitioned, or chromatographically resolved; and the assay may ultimately have received a preparation whose composition differs markedly from the source material. Chemical identity is therefore not an accessory to biological activity. It is part of the evidential definition of the object to which the activity claim belongs. This article uses evidential

object to mean the material or chemical entity directly supported by the observation at issue. That term deliberately separates what investigators handled or measured from broader labels that may be attached to it retrospectively.

The first provenance layer is taxonomic and source identity. Ethnopharmacological reporting standards require attention to nomenclature, collection context, source documentation, and voucher or equivalent traceability so that later investigators can know what biological material a report concerns [2]. These requirements establish an indispensable starting point, but they do not imply that a taxonomically correct specimen has a single invariant chemical composition. Taxonomic identity answers which organism was represented; it does not, by itself, specify which organ, developmental state, extraction procedure, chemical profile, or isolated constituent generated a downstream observation. Treating those distinct questions as one "identity" variable encourages evidence to travel farther than the underlying measurements justify. The problem is especially important when literature synthesis joins reports that share a species name but differ in organ, extraction solvent, processing history, fractionation, or analytical resolution. Apparent agreement across such studies may represent genuine robustness, but it may also result from collapsing unlike test articles under a common botanical heading.

The problem becomes visible in commercial and processed botanical materials, where declared identity and measured composition can diverge. Chemical-authentication studies summarized across commercial herbal products document substitution, adulteration, and substantial variation in detected phytochemical patterns [3]. Such findings do not justify assuming that every labeled product is unreliable. They show instead that label identity, botanical identity, and measured chemical composition are different evidence claims. Processing can also alter detectability, so disagreement between a label, DNA result, and chemical profile is not automatically resolved by privileging one modality. The analytical target and the material state must be specified before an apparent conflict can be interpreted.

Extract research sharpens the distinction further. The ConPhyMP guidance treats the extract used in pharmacological or toxicological research as an object requiring explicit preparation and chemical characterization rather than as an interchangeable surrogate for the plant from which it originated [4]. This article extends that logic into a proposed provenance-centered taxonomy. Its purpose is not to rank species, extracts, fractions, or compounds by intrinsic scientific worth, but to separate the evidential objects they represent and to define when a biological claim may, or may not, be transferred between them. The governing proposition is that biological evidence is initially local to the tested material. Broader attribution requires a defensible provenance bridge rather than a shared species name or presumed continuity of composition.

Pharmacognostic identity as an evidence problem

Species authentication is necessary when a claim depends on organismal identity, but molecular confirmation has a bounded scope. DNA barcoding, species-specific assays, next-generation sequencing, and related approaches can support species assignment in herbal materials, while marker resolution, reference-database coverage, DNA quality, and processing can constrain the inference [5–7]. A molecular result therefore answers a taxonomic question under specified methodological conditions. It does not directly measure the concentrations, relative abundance, or structural identity of the metabolites that entered an assay. Conversely, failure to detect expected DNA in a heavily processed preparation need not establish chemical absence. Taxonomic and chemical evidence should consequently be treated as complementary dimensions rather than interchangeable tests of a single undifferentiated identity. This distinction also prevents an apparently precise species call from functioning as a surrogate measurement for chemistry. The stronger the downstream claim depends on particular constituents or constituent ratios, the weaker that substitution becomes unless chemical evidence accompanies the taxonomic result.

Chemical fingerprinting addresses a different evidential object. Spectroscopic or chromatographic profiles combined with chemometrics can discriminate botanical materials and support authenticity or quality evaluation when suitable reference sets and analytical designs are used [8]. What is established, however, is similarity or separation in a measured multivariate chemical space. The resulting class assignment remains conditioned by extraction, platform, preprocessing, reference composition, and natural variability. A fingerprint can be highly informative without being a complete inventory of composition, and profile similarity cannot automatically establish the identity of every constituent. In the taxonomy developed here, profile evidence therefore sits between material provenance and exact structural assignment rather than replacing either one.

Plant part introduces a material boundary even before extraction. Comparative profiling of leaves, stems, and flowers of *Rumex usambarensis* demonstrated organ-dependent metabolite patterns accompanied by differences

in measured bioactivities [9]. The study is a direct example rather than a universal estimate of organ effects, but it exposes the logical problem: evidence obtained from one part of a species cannot be silently converted into evidence for another part merely because the binomial name is unchanged. Plant-part provenance should remain attached to the tested object, particularly when traditional use, extraction yield, constituent distribution, or biological testing is part specific.

Material identity can also be disrupted after collection. Quality problems involving medicinal plants and herbal products may arise through sourcing, substitution, contamination, storage, or other supply-chain processes [10]. Their prevalence and causes vary by market and product, but the interpretive consequence is general: provenance is a chain, not a label. A study that authenticates an upstream source does not automatically authenticate every downstream material state. Pharmacognostic identity becomes an evidence problem precisely because each transformation can preserve some identity dimensions while changing, obscuring, or severing others. The appropriate response is not to demand one universal authentication method, but to match the method to the identity dimension being claimed and to state which dimensions remain untested.

Levels of material and chemical provenance

The chemical side of provenance begins below the level of a named plant or preparation. LC-MS/MS molecular networking can organize related spectral features, compare sample patterns, and assist metabolite annotation or botanical authentication [11]. These operations are valuable because they preserve relationships among measured features, yet an analytical feature is not synonymous with a compound whose complete structure is known. A peak, ion feature, spectral cluster, library match, and structurally established natural product represent progressively different claims. Provenance-aware interpretation must keep the measured signal linked to the sample in which it occurred while keeping annotation confidence separate from material identity. This produces two simultaneous coordinates: where the signal came from and what the signal is believed to represent. Confusing those coordinates is one route by which an abundant ion in a fraction can later appear in prose as though a structurally established constituent had been directly measured.

Metabolomics operates at the profile level. In medicinal-plant research it can characterize multicomponent chemical variation and support quality evaluation, but the observed profile is conditioned by sample preparation, analytical platform, preprocessing, and annotation workflow [12, 13]. Accordingly, the relevant evidential statement is not that a species possesses one fixed "metabolome," but that a specified material produced a specified analytical profile under stated conditions. This distinction matters for transfer: two preparations may be taxonomically concordant yet analytically different, while two profiles may share major markers without establishing equivalence of every constituent. Profile-level evidence is therefore informative precisely when its methodological boundaries remain visible.

Those boundaries reflect biology as well as instrumentation. Plant metabolomics has revealed substantial metabolic diversity associated with tissue, genotype, development, and environment [14]. Such variation does not make taxonomy irrelevant; taxonomic assignment remains a crucial constraint on plausible chemistry. It does mean that species identity cannot logically serve as an invariant chemical fingerprint. The proposed provenance logic therefore treats taxon-to-chemistry transfer as conditional. Conserved markers may support authentication in appropriate contexts, whereas variable constituents, abundance patterns, and environmentally responsive metabolites require evidence tied more closely to the sampled material.

Fractionation creates another discontinuity. Bioactivity-based molecular networking illustrates how changes in activity across fractions can be associated with molecular features to prioritize candidate active constituents [15]. The inferential value is fraction resolved: a fraction has a composition distinct from its parent extract, and correlated features within active fractions remain candidates rather than automatically causal molecules. Co-elution, correlated abundance, multiple active constituents, or assay-specific effects can all preserve an activity pattern without identifying a single active principle. An isolated material, when eventually obtained, is yet another material state; whether its complete chemical structure is established is a separate question of analytical evidence. These distinctions are consolidated in **Table 1** by separating the material object under investigation from the chemical claim that can legitimately be attached to it.

Table 1. Distinguishing material provenance from chemical evidence states in natural-product research

Provenance or evidence state	What is directly identified	Legitimate evidential scope	Boundary against over-transfer

Species/source material	Taxon and documented source	Organismal provenance	Does not fix plant part or composition
Plant part/material form	Organ or defined physical material	Part-specific test object	Does not authorize transfer to other organs/forms
Extract	Preparation produced by a stated extraction	Extract-specific composition and activity	Not interchangeable with source plant or another extract
Fraction	Composition after a defined separation	Fraction-specific chemistry and assay response	Activity does not identify a single causal constituent
Feature/profile/annotation	Measured signal, pattern, class, or candidate identity	Method-conditioned chemical evidence	Not equivalent to complete structural proof
Isolated material	Separated constituent as a physical test object	Isolate-specific observations	Isolation status does not itself specify structural certainty

Note: The separation of these states is the proposed analytical organization used in this article. Material provenance and chemical-identification confidence are related but non-equivalent dimensions.

Proposed provenance-centered taxonomy

The proposed taxonomy treats provenance as a nested description of the object that generated evidence, while keeping chemical-identification confidence on a parallel axis. This avoids a common category error in which increasing analytical resolution is mistaken for a change in material provenance. Feature-based molecular networking, for example, can retain quantitative sample-level features while organizing MS/MS relationships [16]. The feature remains traceable to an extract or fraction, but it does not become a confirmed compound merely because it occupies a well-connected spectral neighborhood. The first rule of the taxonomy is therefore preserve the material path: species/source → plant part or material form → extract → fraction → isolated material, recording only stages actually established rather than reconstructing missing steps by assumption. Missing provenance is recorded as missing provenance, not converted into presumed continuity.

The second rule is preserve source-to-structure linkage without collapsing intermediate states. The LOTUS initiative demonstrates the value of curated, referenced relationships between natural-product structures and source organisms [17]. The taxonomy proposed here extends that provenance principle conceptually by asking, where evidence permits, which plant part, preparation, extract, fraction, or isolate connects the organismal source to the chemical claim. This extension is not presented as existing LOTUS functionality or as a universally recoverable historical record. Older publications may omit intermediate details, and retrospective reconstruction can remain incomplete. In such cases, “unknown” is a valid provenance state and is preferable to an inferred continuity that the source does not document.

The third rule is separate contextual plausibility from direct chemical identification. Taxonomic information can improve confidence in metabolite annotation by favoring candidates consistent with known biological occurrence [18]. That use of provenance is scientifically valuable, but taxonomic plausibility remains supporting evidence. It can raise or lower confidence in a candidate without converting an annotation into experimental structural proof. The same distinction applies in the opposite direction: an unusual chemical assignment should not be rejected solely because existing occurrence databases lack the organism–compound relationship, because database coverage is incomplete and genuinely novel chemistry remains possible.

The fourth rule is grade the chemical claim independently of the material state. Modern computational MS/MS and MS/NMR approaches can provide compound-class assignments or candidate structures with graded confidence, but these outputs remain distinct from definitive experimental establishment of an isolated natural product’s complete structure [19–21]. Accordingly, the proposed chemical-evidence axis distinguishes at least measured feature, reproducible profile relation, compound-class assignment, candidate structural annotation, and structurally established identity. The precise analytical route can vary; the taxonomic point is that each label describes what is known chemically, not what physical material was tested. An extract may contain a strongly annotated feature, and an isolate may still carry residual structural uncertainty.

The final rule is do not equate isolation with correctness of structural assignment. Critical analysis of natural-product structural misassignments shows that even isolated small molecules can require later structural revision when spectral interpretation, stereochemical assignment, or other evidence has been overextended [22]. These examples do not establish a general misassignment rate, but they demonstrate why “isolated compound” must remain a material-state descriptor rather than a synonym for “chemically certain molecule.” The taxonomy

therefore produces a provenance vector rather than a single authenticity score: a claim may be strong at the species level, uncertain at the plant-part level, well characterized at the extract level, fraction resolved, and still only candidate-level at the structural level. Biological interpretation should inherit exactly that pattern of certainty, not a simplified label of "identified natural product."

Evidence transfer across pharmacognostic levels

The taxonomy becomes consequential when evidence is moved from one provenance level to another. Mass-spectrometric authentication of botanical supplements can support the presence, absence, or pattern of chemical markers, but botanical inference depends on marker specificity, processing, matrix effects, and the reference context against which the signal is interpreted [23]. A detected metabolite can therefore strengthen a species or material claim only when a justified bridge exists between that metabolite and the claimed source. The reverse is equally important: a verified botanical source does not establish the abundance of a marker in every preparation derived from it. Evidence transfer is thus conditional rather than automatic, and its conditions should be stated rather than hidden inside a shared botanical name.

Orthogonal authentication studies make this non-equivalence visible. In commercial *Hypericum perforatum* products, DNA metabarcoding and chemical methods provided different forms of information because processing, molecular detectability, and chemical composition affected the modalities differently [24]. Such discordance should not automatically be framed as a contest in which one method must be "right." The more defensible interpretation asks which identity dimension each method measured. Taxonomic evidence can remain strong while chemical composition is uncertain, and chemical-marker evidence can remain interpretable when recoverable DNA is limited.

The same principle applies when multiple methods agree. *Echinacea* products assessed by DNA metabarcoding and chromatographic profiling illustrate how taxonomic detection and chemical fingerprints can complement one another without becoming one binary authenticity result [25]. Concordance strengthens a composite interpretation only to the extent that each method addresses the relevant provenance question. It does not convert product-level agreement into proof of plant-part history, manufacturing continuity, biological equivalence, or complete constituent identity.

Integrated genetic and NMR assessment of *Garcinia* materials similarly demonstrates that independent taxonomic and chemical evidence can be combined while preserving their separate scopes [26]. The proposed transfer rule is therefore explicit: evidence may move across pharmacognostic levels only through a documented bridge appropriate to the claim. Acceptable bridges may include traceable processing continuity, a validated source-specific marker, an orthogonal chemical/taxonomic match, or direct testing of the downstream material. Absence of such a bridge is not evidence of falsehood; it is a limit on what can legitimately be inferred.

Table 2 summarizes the permitted and non-permitted forms of transfer that follow from this distinction.

Table 2. Proposed evidence-transfer rules across pharmacognostic levels

Source evidence	Intended transfer	Bridge required	Claim remaining unsupported without the bridge
Species identity	Plant-part chemistry	Defined organ plus part-specific evidence	All organs share the measured chemistry
Plant part	Extract composition	Traceable extraction and extract characterization	Extract reproduces source material unchanged
Extract	Fraction activity	Defined fractionation and fraction-resolved assay	Crude-extract activity identifies the same active constituents
Fraction	Isolated constituent activity	Isolation plus direct or orthogonal activity confirmation	Correlated fraction feature is the causal molecule
Chemical marker/profile	Botanical identity	Demonstrated specificity in the relevant processed matrix	One marker establishes complete botanical provenance
Candidate annotation	Confirmed structure	Appropriate confirmatory structural evidence	Annotation confidence equals definitive molecular identity

Note: These transfer rules are proposed for evidence organization. They do not constitute validated performance criteria or a regulatory decision framework.

Figure 1 integrates the provenance levels, chemical-evidence states, transfer gates, and reporting boundaries into a single manuscript-derived architecture.

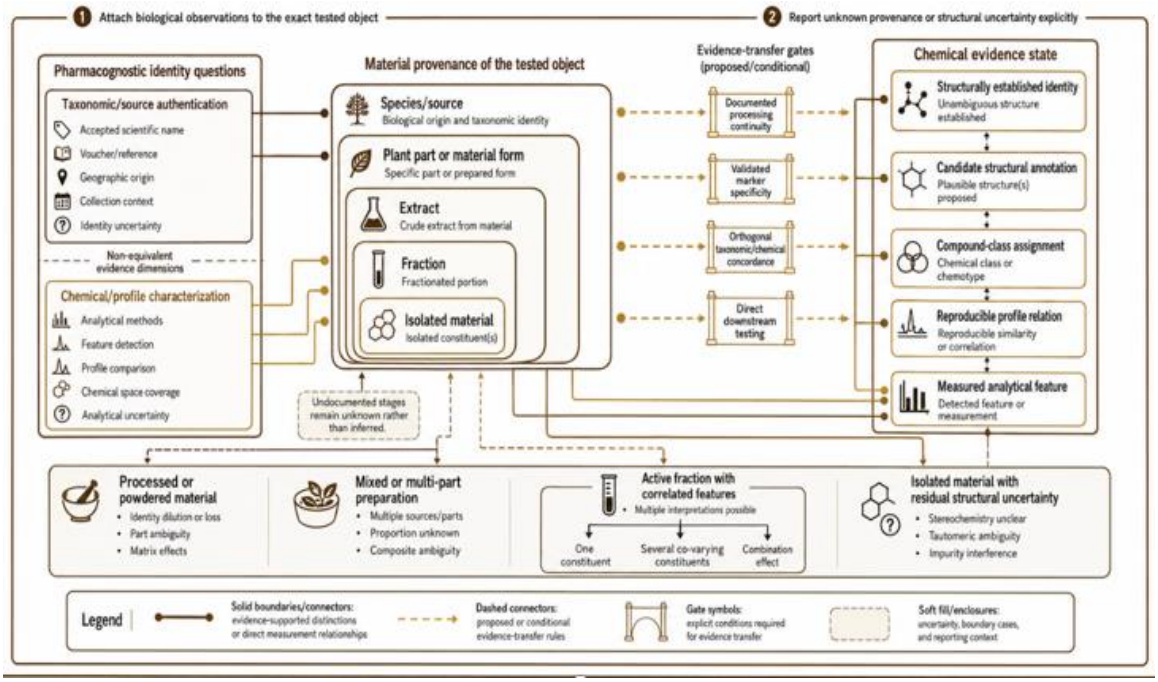

Figure 1. Provenance-preserving transfer of natural-product evidence across material and chemical identity states

Applications and boundary cases

Material form is a practical boundary because processing can change both authenticity risk and what an analytical method can recover. In market samples of *Withania somnifera*, DNA-barcoding analysis reported greater adulteration among powders than among root samples in the studied context [27]. That result should not be generalized into a universal rule that powders are unreliable or intact roots are authentic. Its value for the taxonomy is narrower: evidence about one material form should not automatically validate another when processing can alter source traceability, opportunities for substitution, or analytical accessibility.

Orthogonal validation can reduce some uncertainty without eliminating the provenance structure. Genome-skimming and NMR chemical fingerprinting were jointly used to assess Sarsaparilla identity and purity, illustrating how genomic and chemical evidence can reinforce one another while remaining distinct measurements [28]. Under the proposed taxonomy, such concordance increases confidence across more than one dimension, but it does not establish biological activity or therapeutic equivalence unless those outcomes are directly tested.

Mixed or multi-part preparations are harder cases because the material object itself may not fit a single plant-part label. Organ-dependent metabolite and bioactivity differences demonstrate why forcing such materials into an unspecified species-level category can erase relevant variation [9]. The proposed solution is not to invent a dominant part retrospectively, but to record the mixture or uncertainty as part of provenance. The same principle applies to historical remedies when source descriptions are incomplete: an unknown field should remain unknown rather than being filled by modern assumptions.

Fractionation creates a different ambiguity. A molecular feature that tracks with active fractions is evidence for prioritization, not proof that the feature represents the sole causal agent [15]. Co-elution, multiple active constituents, or activity emerging from combinations remain plausible until further testing. At the isolated-material level, structural certainty also remains separable from biological observation because natural-product structures can be revised after initial assignment [22]. Difficult cases therefore do not invalidate provenance classification; they are where it is most useful, because the taxonomy can preserve uncertainty rather than resolving it by nomenclatural convenience. A related case is the multi-botanical preparation: even when every declared species is correctly detected, the tested object remains the mixture rather than a set of independently demonstrated single-species effects. Provenance should therefore preserve mixture composition, processing history, and the level at which any chemical or biological observation was actually obtained.

Implications for research reporting

A provenance-centered report should identify the object actually tested before describing what that object did. For extract-based pharmacology, this means recording the source material, relevant plant part, extraction conditions, and chemical characterization with enough detail to define the preparation [4]. The proposed reporting principle is proportional rather than maximalist: not every experiment requires exhaustive metabolomics, but every biological claim should be anchored to a test article whose identity is adequate for that claim. If an activity belongs to a fraction, the fraction should remain named; if it belongs to an isolate, the isolate's structural-confidence basis should be stated separately from its material provenance.

Digital natural-product records should preserve the same distinction. Referenced structure–organism links, as demonstrated by LOTUS, show the utility of retaining explicit provenance instead of storing natural products as context-free structures [17]. Where the literature permits, records could additionally retain plant part, material form, extraction, fractionation, and evidence-status fields. This is proposed as a data-organization extension, not as a claim that such metadata can always be reconstructed retrospectively. Legacy reports may omit critical steps, and uncertainty should be represented explicitly rather than converted into inferred continuity.

The reporting consequence for biological claims is straightforward: the result attaches first to the characterized object that entered the assay. Best-practice phytopharmacological guidance supports the broader need for reproducible, adequately defined research materials [1]. The taxonomy adds a claim-matching rule: a species-level statement, extract-level activity, fraction-level association, and isolated-compound effect should not be merged merely because they are linked by a shared natural-product narrative. Transfer is permissible when the report supplies a defensible bridge; otherwise, broader wording should remain qualified.

Structural reporting requires the same discipline. Documented cases of natural-product structural revision demonstrate that isolation does not eliminate interpretive error [22]. Authors should therefore report material state and structural-certainty status independently, especially when identification relies substantially on spectral annotation, computation, or incomplete stereochemical evidence. This separation also improves literature reuse: a later database, review, or pharmacological study can distinguish what was physically isolated from what was chemically established and can update one dimension without rewriting the other. Provenance-aware reporting is therefore less about adding labels than about preventing uncertainty from disappearing as evidence moves downstream.

A practical report can implement this without converting every article into an authentication study. At minimum, the provenance description should make clear which taxon was intended or demonstrated, which plant part or material form was used, how the tested preparation was produced, whether further fractionation occurred, and what analytical statement supports any named chemical entity. When one of these elements is unavailable, the absence itself should be visible. This prevents later reviewers or databases from mistaking an omitted field for an established one and allows evidence to be reclassified when stronger authentication or structural information becomes available.

Conclusion

Natural-product evidence is often organized around names that appear more stable than the materials and measurements beneath them. A species name can refer to several organs; a plant part can generate chemically different extracts; an extract can be partitioned into fractions whose activities are composition specific; and an isolated material can still carry uncertainty about exact structure. Treating these states as interchangeable allows biological claims to drift away from the object that actually generated them.

This article proposes a provenance-centered taxonomy that separates five material states—species/source, plant part or material form, extract, fraction, and isolated material—from a parallel axis of chemical-evidence states. The central interpretive rule is that biological evidence is initially local to the tested object. Transfer to another pharmacognostic level requires an explicit and defensible bridge, such as documented processing continuity, validated marker specificity, orthogonal authentication, or direct downstream testing. Unknown or unresolved provenance should remain visible rather than being repaired by assumption.

The taxonomy is intended as an organizing framework, not a validated scoring system, causal model, regulatory standard, or guarantee of reproducibility. It does not imply that every study requires the same analytical depth, that taxonomy is chemically uninformative, or that discordant authentication methods necessarily contradict one another. Its value lies in forcing the evidential question to precede the biological one: what exactly is known about the material, and at which level is it known?

Future evaluation should test whether independent readers can apply the categories reproducibly, whether provenance-aware reporting reduces unsupported cross-level attribution, and whether the framework remains useful across raw botanicals, processed products, complex extracts, fractions, and isolated natural products. Until such validation is available, the taxonomy should be treated as a proposed discipline for keeping chemical identity, material provenance, and biological interpretation aligned. Its strongest claim is therefore procedural: natural-product evidence should become broader only when the provenance and analytical justification for that broader inference are visible. That discipline preserves useful uncertainty, makes disagreements easier to localize, and gives later experimental work a clearer account of which identity link requires confirmation.

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