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Research

Genetic and environmental drivers of intraspecific variation in foliar metabolites in a tropical tree community

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Summary

- Plant interactions with abiotic and biotic environments are mediated by diverse metabolites, which are crucial for stress response and defense. These metabolites can not only support diversity by shaping species niche differences but also display heritable and plastic intraspecific variation, which few studies have quantified in terms of their relative contributions.
- To address this shortcoming, we used untargeted metabolomics to annotate and quantify foliar metabolites and restriction-site associated DNA (RAD) sequencing to assess genetic distances among 300 individuals of 10 locally abundant species from a diverse tropical community in Southwest China. We quantified the relative contributions of relatedness and the abiotic and biotic environment to intraspecific metabolite variation, considering different biosynthetic pathways.
- Intraspecific variation contributed most to community-level metabolite diversity, followed by species-level variation. Biotic factors had the largest effect on total and secondary metabolites, while abiotic factors strongly influenced primary metabolites, particularly carbohydrates. The relative importance of these factors varied widely across different biosynthetic pathways and different species.
- Our findings highlight that intraspecific variation is an essential component of community-level metabolite diversity. Furthermore, species rely on distinct classes of metabolites to adapt to environmental pressures, with genetic, abiotic, and biotic factors playing pathway-specific roles in driving intraspecific variation.

Introduction

The metabolome, the suite of small organic compounds, or metabolites in an organism, represents a deep and diverse pool of functional trait variation that mediates plant interactions with the environment (Walker *et al.*, 2022). Plant metabolites mediate abiotic stress responses and adaptations to drought, heat, freezing temperatures, and ultraviolet light (Tegelberg *et al.*, 2001; Defossez *et al.*, 2021; Volf *et al.*, 2023). By acting as attractants and defenses, they also shape the host ranges of natural enemies such as herbivores and pathogens (Salazar *et al.*, 2016; Endara *et al.*, 2017) and mutualists such as pollinators (Rivest *et al.*, 2024). The biosynthesis of metabolites requires energetic investment from the plant; hence, metabolites contribute to fundamental trade-offs in resource allocation that define alternative defense syndromes (Kursar & Coley, 2003) and life-history strategies (Coley *et al.*, 1985). Finally, because of their role as functional traits, variation in metabolites is associated with species distributions across environmental gradients (Defossez *et al.*, 2021; Volf *et al.*, 2023) and individual performance (Forrister *et al.*, 2019).

Plant functional ecology seeks to understand individual performance as a function of traits and to extrapolate such relationships to understand variation in species distributions and abundances and community diversity over space and with respect to environmental gradients (Yang *et al.*, 2018). It is commonplace to represent individuals of a species using species mean trait values, which has been used to reveal important insights into species-level trade-offs (Wright *et al.*, 2004) and broad differences in communities (Sedio *et al.*, 2018). However, the distribution and co-occurrence of species are the result of the successes

and failures of individual plants, which may be best understood in the context of the phenotype of individuals (He *et al.*, 2022; Rubio & Swenson, 2024). Recent studies have demonstrated the importance of intraspecific trait variation (ITV) in trait-based community ecology (Violle *et al.*, 2012; Siefert *et al.*, 2015; Kuppler *et al.*, 2020) and that accounting for intraspecific variation improves predictive power for tree demography (Yang *et al.*, 2018, 2021; Asefa *et al.*, 2021).

Techniques that seek to identify, classify, and quantify the vast diversity of metabolites present in a tissue or organism, known as untargeted metabolomics (Di Minno *et al.*, 2021), have advanced dramatically in the past decade, with exciting implications for plant ecology (Sedio, 2017; Sun *et al.*, 2024). Untargeted metabolomics allows for comprehensive profiling of metabolic diversity without prior knowledge of specific compounds, making it particularly valuable for studying ecological interactions. Studies integrating metabolomics and plant community ecology have provided new insights into plant–herbivore interactions (Forrister *et al.*, 2019; Wang *et al.*, 2023; Sun *et al.*, 2024), community assembly (Sedio *et al.*, 2018; Endara *et al.*, 2022; Müller & Junker, 2022), and ecosystem processes (Sardans *et al.*, 2011; van Dam & van der Meijden, 2011) across environmental gradients (Defossez *et al.*, 2021; Volf *et al.*, 2023). However, a key feature of untargeted metabolomics data is that it is difficult to compare across species because of the large degree of divergence in phytochemical composition, the small number of shared metabolites even among congeneric species, and challenges in metabolite annotation and detection sensitivity (Sedio *et al.*, 2017; Forrister *et al.*, 2023). This extreme disparity in composition has necessitated the development of new analytical methods for comparative metabolomics, such as similarity metrics that account for the structural similarity of unique metabolites (Sedio *et al.*, 2017). It has also resulted in a general sense that since interspecific metabolite variation is substantial, quantifying intraspecific metabolite diversity may be of lesser importance for comparative metabolomics in community ecology (Sedio *et al.*, 2017).

Despite the mounting evidence of vast interspecific variation, plant metabolites are also well known to exhibit substantial within-species variation, and this is likely critically important for ecological investigations (Rubio & Swenson, 2024). Metabolomes of individual plants respond dynamically to variations in the environment (Wang *et al.*, 2019; Wetzel & Whitehead, 2020). For example, Huberty *et al.* (2020) showed that plant-induced changes in soil can modify the metabolomes of plants growing in those soils subsequently, highlighting how plant–soil feedbacks may significantly contribute to the often unexplained intraspecific variation in plant chemical composition. Some intraspecific metabolite variation is clearly linked to genetic differences, as in *Populus tremuloides*, where genotypic variation drives chemical heterogeneity (Kroymann, 2011). Furthermore, genetic variation in *Pinus sylvestris* influences terpene diversity (Iason *et al.*, 2005). Such variation may have significant fitness effects, as within-species chemical variation shows observable effects on herbivorous caterpillars in *Piper* (Glassmire *et al.*, 2016). Taken together, a growing body of work suggests that intraspecific metabolite variation, driven by genetic variation or responses to the environment, may be essential to consider because of its functional consequences for plant performance.

Untargeted metabolomics holds great promise for improving mechanistic and predictive power in ecology by integrating metabolites, physiology, and fitness (Kessler & Kalske, 2018; Müller & Junker, 2022; Walker *et al.*, 2022). Unlike traditional unidimensional traits (e.g. specific leaf area) that measure static phenotypic compromises, plant metabolomes function as high-dimensional phenotypic integrators: hundreds of covarying metabolites dynamically encode organismal responses through biochemical networks, simultaneously reflecting genetic constraints, environmental plasticity, and biotic interactions (Kessler & Kalske, 2018). However, the extreme variability of plant metabolomes poses analytical challenges. While traditional traits rely on direct measurement protocols, metabolomics requires multistep computational pipelines—including peak detection, retention time alignment, batch correction, and normalization—to transform raw LC-MS data into feature lists. These features can then be annotated via spectral databases or analyzed through molecular networks to resolve compound association patterns. By quantifying chemical diversity indices or similarity metrics, metabolomic variation can be linked to ecological processes. Addressing the relative degree of intra- vs interspecific metabolite variation and how this variation is linked to underlying genetic and environmental factors is crucial for understanding when, where, and why quantifying intraspecific metabolite diversity is useful. This is particularly important as untargeted metabolomics, unlike functional trait data, can be logistically and financially prohibitive for large numbers of individuals.

Here, we present the first metabolomic study of genetic and environmental drivers of intraspecific metabolite variation in tree species co-occurring within a tropical forest community. We use untargeted metabolomics based on high-resolution mass spectrometry to quantify and classify metabolites, alongside RAD sequencing to assess genetic distances among 30 individuals of each of 10 locally abundant species in a species-rich tropical moist forest in Southwest China. In addition, we used measurements reflecting soil, light, neighborhood crowding, and herbivory to quantify variation in the abiotic and biotic environment experienced by individual trees within a permanent 20-ha forest dynamics plot and evaluated the relative contributions of genes and the abiotic and biotic environment to intraspecific metabolite variation to address the following questions: (i) Is intraspecific metabolite variation important relative to overall variation within a community? (ii) What is the relative importance of genetic diversity, abiotic environment, and biotic environment in contributing to intraspecific metabolite variation? (iii) Does the relative importance of these factors vary among metabolites from different biosynthetic pathways with broad differences in function?

Materials and Methods

Study site

This study was conducted in a 20-ha tropical seasonal rainforest dynamics plot (FDP) located in Xishuangbanna, Southwest

China (21°36′42″–58″N, 101°34′26″–47″E; Supporting Information Fig. S1). The plot was established in 2007 within the Xishuangbanna National Nature Reserve and is dominated by *Parashorea chinensis* H. Wang (Dipterocarpaceae). The mean annual temperature is 21.8°C (Cao *et al.*, 2006). Influenced by the monsoon climate, the region receives an annual rainfall of 1493 mm, 84% of which falls during the wet season (May–October; Yang *et al.*, 2021). The elevation ranges from 708 to 869 m above sea level, contributing to significant habitat heterogeneity (Lan *et al.*, 2009). Following the standard protocols for FDPs from Condit (1998), all free-standing woody stems with a diameter at breast height (DBH) of at least 1 cm were identified, mapped, tagged, and measured every 5 yr. The initial census in 2007 recorded 468 species and 95 946 individuals, and three re-censuses have been completed to date. Further details on the climate, geology, and flora of the plot are available in Cao *et al.* (2008).

Focal species selection

The main objective of this study was to investigate intraspecific variation in foliar metabolites and assess the relative contributions of genetic diversity and environmental factors to this variation. To achieve this, we strategically selected 10 tree species, considering factors such as abundance, habitat heterogeneity, and representation across different life stages. First, we focused on common species with population sizes over 500, based on census data from 2017, as larger populations tend to harbor greater genetic diversity, facilitating local adaptation and functional differentiation (Raabová *et al.*, 2015). Second, priority was given to habitat generalists. This selection minimized the confounding effects of environmental factors and genetic influences caused by dispersal limitation. We also prioritized species exhibiting low gene flow and spatial autocorrelation in the environment. However, the small plot size and limited environmental variation make it unlikely that strong selective gradients or limited gene flow would generate strong genotype–environment correlations. Additionally, we selected species that represented a range of cohort stages, from small to large individuals (Yang *et al.*, 2014). This approach enabled a comprehensive assessment of ITV and genetic differentiation across developmental stages. We sampled 30 individuals per species, evenly distributed across the quadrats where they occurred, resulting in 300 individuals from 10 tree species (Table S1).

Leaf sampling and processing

From each focal individual, three to five young, fully expanded leaves were randomly collected. The leaf samples were immediately placed in liquid nitrogen to preserve DNA and metabolites and stored in a −80°C freezer at the laboratory. Three branches were randomly selected from different directions, with each containing more than 10 leaves. Ten leaves from each branch were collected sequentially from top to bottom to accurately assess herbivore damage.

Restriction site-associated DNA sequencing (RAD-Seq) was performed to obtain high-resolution population genomic data (detailed methods see Methods S1). DNA was extracted using a modified cetyltrimethylammonium bromide (CTAB) method (Doyle & Doyle, 1990), and samples were sent to BGI-Wuhan (Wuhan, China) for library construction and sequencing. A non-targeted metabolomic approach based on ultra-high-performance liquid chromatography–tandem mass spectrometry (UHPLC–MS/MS) was used for metabolite analysis, following the protocols of Sedio *et al.* (2018, 2021), with slight modifications to suit our laboratory equipment.

Approximately 250 mg of finely ground leaf material was mixed with 1800 µl of 90 : 10 methanol : water extraction solvent (pH 5). The mixture was shaken at 2.81570 ***g*** for 5 min, followed by 0.14985 ***g*** for 8 h at 4°C. After shaking, samples were centrifuged at 19 693 ***g*** for 30 min at 4°C, and the supernatant was collected. Methanol was evaporated using a vacuum centrifuge concentrator, reducing the volume to about one-third, leaving mostly the water phase, and the samples were freeze-dried for 24 h. The dried material was reconstituted in 1000 µl of extraction solvent, filtered through a 0.22 µm Millipore filter, and transferred to 2 ml brown chromatographic vials. Instrumental methods for metabolite detection were modified from Sedio *et al.* (2018, 2021) for the use of an Agilent 1290 UPLC/Q-TOF using a GOLD aQ analytical column (250 mm × 4.6 mm, 5-µm particle size). Chromatographic separation was achieved with a solvent gradient using ultrapure water (Buffer A) and acetonitrile (MeCN, Buffer B), starting at 20% Buffer B for 20 min, then linearly increasing to 100% over 30 min. For electrospray ionization in positive ion mode, the gas temperature was set at 350°C with an 8 l min^{-1} gas flow. Tandem mass spectrometry (MS/MS) was conducted using time-of-flight (TOF) MS, with a fragmentation voltage of 135 V, skimmer voltage of 65 V, and Vpp of 750 V. The MS1 and MS2 spectra were acquired for mass-to-charge ratios (*m/z*) of 100–1700 and 20–1700, respectively, with a 1 spectrum/second acquisition rate. Collision energy was adjusted between 10 and 50 eV for optimal metabolite fragmentation and structural characterization.

Environmental measurements

To quantify the effects of abiotic factors on intraspecific metabolite variation, we used data on 10 soil variables and the light environment, which have been found to influence plant performance and species distributions at our site (Hu *et al.*, 2012; Yang *et al.*, 2014; Song *et al.*, 2018). Soil variables were recorded at 756 points within the plot and included total nitrogen (TN), total phosphorus (TP), total potassium (TK), total carbon (TC), available nitrogen (AN), extractable phosphorus (AP), extractable potassium (AK), bulk density, pH, and moisture (Hu *et al.*, 2012). We used canopy openness in each 20 m × 20 m quadrat as a proxy for the light environment (Wang *et al.*, 2023). This was done by capturing hemispherical photographs with a digital camera, which were then analyzed using the Gap Light Analyzer v.2.0 software. The software calculated the canopy gap fraction, indicating the portion of each image that was open and nonvegetated (Frazer *et al.*, 2000).

To fully assess the influence of biotic factors on intraspecific metabolite variation, we quantified the effects of neighborhood

size and herbivore damage. The neighborhood crowding index (NCI; Canham *et al.*, 2006) was used to quantify the impact of neighboring trees on 300 focal individuals. Specifically, the NCI for a focal tree (i) was calculated as the sum of contributions from all neighboring trees within 15 m (Yang *et al.*, 2014, 2021) around the focal tree. The contribution of a neighboring tree (j) is modulated by its DBH and distance from the focal individual as per the following formula:

$$\mathrm{NCI}_i = \sum_{j=1, i\neq j}^{n_j} \frac{\mathrm{DBH}_j^2}{\mathrm{dist}_{ij}^2}$$

where DBH_j is the diameter at breast height of the neighboring tree, and dist_{ij} is the Euclidean distance between the focal and neighboring trees.

To accurately assess herbivore damage, we scanned 30 leaves of each individual using an Epson scanner (Epson Co., Beijing, China). We distinguished different damage types using the 'Guide to Insect (and Other) Damage Types on Compressed Plant Fossils' (Labandeira *et al.*, 2007) and our field expertise, disregarding fungal and mechanical damage (Sun *et al.*, 2024). Adobe Photoshop (Adobe System Inc., USA) was used to outline missing leaf edges and blacken visible damages for analysis. Leaf damage quantification was performed using ImageJ software (v.1.47), calculating the remaining and original leaf area as per Abramoff *et al.* (2004). The leaf area lost to herbivory was calculated by subtracting the remaining area from the original leaf area. We calculated the leaf area loss ratio, defined as the leaf area lost to herbivory divided by the original leaf area (Andrew *et al.*, 2012).

Genetic data processing

Genetic diversity was analyzed by calculating pairwise genetic distances among individuals to generate a genetic distance matrix (detailed methods see Methods S2). This process included the *de novo* assembly and SNP calling using the Stacks 2.5 pipeline (Rochette & Catchen, 2017). Low-quality reads and those with potential adapter contamination were filtered, and SNPs were called using the 'population' module. Only loci present in at least two species and with < 20% missing data were retained. Genetic distances were quantified using the identity-by-state matrix in PLINK (Purcell *et al.*, 2007). We performed a principal component analysis (PCA) on the genetic distance matrix to generate genetic eigenvectors and selected the first three axes for downstream analyses (Swenson, 2014). These axes summarize the most informative genetic differences, enabling efficient incorporation of genetic diversity into our models.

Metabolomic data preprocessing

We started by converting raw mass spectrometry files using MSConvert, converting .d files to .mzXML format with 64-bit binary encoding precision and zlib compression. We applied Peak Picking with the Vendor's algorithm, limiting MS levels to 1–2. For mass data processing, we used MZmine (v.3.9.0; Schmid *et al.*, 2023) and adjusted the parameters to match the instrument specifications. Mass detection was conducted for MS1 and MS2 using a centroid mass detector (MS1 noise = 1×10^3, MS2 noise = 0). Chromatograms were built using the ADAP chromatogram builder (minimum scan group size = 4, minimum group intensity = 1×10^3, minimum highest intensity = 2×10^3, and m/z tolerance = 0.005 m/z or 10.0 ppm). Peaks were deconvoluted with the local minimum resolver algorithm (chromatographic threshold = 90%, minimum search range RT/Mobility = 0.05, minimum relative height = 0.0%, minimum absolute height = 2×10^3, minimum ratio of peak top/edge = 1.8, peak duration range = 0.0–3.0, minimum data points = 4). Isotopes were detected using the 13C isotope filter (m/z tolerance = 0.005 m/z or 10.0 ppm, absolute RT tolerance = 0.1 min, maximum charge = 2). Peaks were aligned using the join aligner method (m/z tolerance = 0.005 m/z or 10.0 ppm, m/z weight = 3, RT weight = 1, absolute RT tolerance = 0.1 min). We exported the feature list for FBMN/SIRIUS and created the spectral file (.mgf) and ion abundance 'quant' table (.csv), as well as the SIRIS/CSI FingerID feature list. Molecular networking was conducted on the GNPS (Wang *et al.*, 2016) platform using the feature-based molecular networking (FBMN) workflow (Nothias *et al.*, 2020), with mass tolerance and network options set to default (Minimum Pairs Cos = 0.6).

For feature annotation, SIRIUS (v.5.8.5) was used to classify compounds (detailed methods see Methods S3) into seven major biosynthetic pathways of origin based on NPClassifier (Kim *et al.*, 2021) using Canopus (Dührkop *et al.*, 2021): carbohydrates and fatty acids, which we defined as primary metabolites; and alkaloids, amino acids and peptides, polyketides, shikimates and phenylpropanoids, and terpenoids, which we classified as secondary metabolites. Primary metabolites are crucial for basic cellular functions like growth and energy production, while secondary metabolites play significant roles in environmental interactions, such as defense and stress adaptation (Wink, 2003). We removed metabolites with Canopus confidence scores ≤ 0.90 for the 'pathway'-level classification. A master table combining quant data and metadata (sample information) was constructed, with compounds from blank samples and those with peak areas < 10 000 removed, a threshold chosen based on data quality considerations, including instrument sensitivity and background noise levels. This dataset supported further downstream analyses.

Statistical analyses

We initiated our analysis by examining the metabolome profiles of 300 individuals across 10 species to characterize the profiles of metabolites within each species, including maximum, minimum, mean values, and standard deviations of metabolite richness among individuals in each species. We also calculated the proportion of these compound features in each biosynthetic pathway for each species. To assess intraspecific variation in metabolite richness, we used Kvålseth's coefficient of variation (^{k}CV)

(Kvålseth, 2017), an improved version of the standard coefficient of variation that accounts for scale. The ^{k}CV is defined as

$$^{k}\mathrm{CV} = \sqrt{\frac{\mathrm{CV}^2}{1 + \mathrm{CV}^2}}$$

where $\mathrm{CV} = \frac{\mathrm{SD}}{\mathrm{mean}}$, quantified the degree of variation within each species.

To identify the sources of variation across different metabolite biosynthetic pathways, we applied a framework from Messier *et al.* (2010) to decompose the variance in metabolite richness across four hierarchical levels: plot, species, life-history stage, and individual trees. This approach was applied using the varcomp function in the R package APE (Paradis & Schliep, 2019). Using the lme function in NLME (Pinheiro *et al.*, 2024), we used a generalized linear model with the Restricted Maximum Likelihood (REML) optimization method to account for hierarchically nested variances, with metabolite biosynthetic pathway treated as a fixed effect. Additionally, we partitioned the dataset into primary metabolites and secondary metabolites, applying the same variance decomposition framework to each subset.

We also used the quant table and network data to calculate chemical structural-compositional similarity (CSCS; Sedio *et al.*, 2017), a method for assessing structural and compositional similarities among sample pairs. Unlike traditional ecological similarity measures such as Bray–Curtis, which focus on compound concentration or ion intensity, CSCS also incorporates molecular structural relationships. This approach evaluates not only shared compounds but also those with similar structures, even if they are not common to both samples. We generated matrices detailing the chemical similarity between all individual pairs sampled. Our analysis covered the entire metabolome, primary metabolites, secondary metabolites, and the seven major biosynthetic pathways, enabling us to quantify CSCS within each of the 10 species.

We compared metabolomic dissimilarities among individuals using nonmetric multidimensional scaling (NMDS) applied to the dissimilarity matrix using the isoMDS function in MASS (Venables & Ripley, 2002). Metabolite dissimilarity was quantified as 1 − CSCS. This analysis reduced the complexity of chemical space to two dimensions for visualization. To statistically assess the significance of interspecific differences in compound composition, we performed a permutational analysis of variance (PERMANOVA) using the adonis2 function in VEGAN (Oksanen *et al.*, 2024). The NMDS and PERMANOVA were applied to the dissimilarity data for the entire metabolome, primary metabolites, secondary metabolites, and seven major biosynthetic pathways. Additionally, we calculated the mean dissimilarity within and across species for each compound category to provide a valuable measure of intra- vs interspecific diversity. For mean interspecific dissimilarity, we performed pairwise comparisons between all species, resulting in 45 unique species combinations. For each combination, the mean dissimilarity was computed based on the dissimilarities between the samples of the two species involved. For mean intraspecific dissimilarity, we calculated the mean dissimilarity within each of the 10 species.

To assess the relative contributions of genetic diversity, abiotic environment, and biotic environment to intraspecific metabolite variation, we also applied PERMANOVA. Abiotic environmental variables were preprocessed by removing factors with correlations greater than 0.6, followed by standardization and PCA, which extracted the first three components explaining over 76% of the total variation (Table S2). Biotic environmental factors, including measures of neighborhood crowding and herbivory damage, were also standardized. Genetic eigenvector processing is detailed in the previous section. We constructed three main models: (1) a model assessing the individual contributions of genetic diversity, abiotic environment, and biotic environment; (2) a model evaluating the interaction between genetic diversity and abiotic environment; and (3) a model evaluating the interaction between genetic diversity and biotic environment. These three models were applied independently to each of the 10 species, with each model evaluated using 10 sets of response variables: overall metabolite dissimilarity, primary and secondary metabolite dissimilarity, and dissimilarity for each of seven major biosynthetic pathways, where each data point represents the dissimilarity between two individuals. Additionally, at the community level (using data from all species), we applied these three models and added a model considering the interaction between biotic and abiotic environments to provide an overall assessment. Metabolite dissimilarity was quantified as 1 − CSCS for each dataset. The explanatory power of each model was assessed by R^2 values, and model significance was determined via 999 permutation tests. All analyses were conducted in R v.4.4.1 (R Core Team, 2024).

Results

Intraspecific variation in foliar metabolites

An analysis of leaf extracts from 300 individuals representing 10 species provided a total of 3146 unique features with biosynthetic pathway predictions with ≥ 0.90 confidence and abundance > 10 000 units in the chromatographic peak area. These compounds had a combined total of 19 586 occurrences across all individuals. Terpenoids and fatty acids were the most prevalent, comprising 24.66% and 24.11% of the total, while polyketides were the least frequent at 5.70% (Fig. S2). Compound richness exhibited substantial intraspecific variation across species (Fig. 1a; Table 1). *Macropanax dispermus* displayed the largest variation; the number of compounds per individual ranged from 14 to 207, with an average of 59 compounds per individual. By contrast, *Baccaurea ramiflora* displayed the least variation, with individual compound counts ranging from 13 to 84 and an average of 39 compounds (Table 1). The coefficient of intraspecific variation (^{k}CV) in compound richness was generally high and exhibited notable variation among species, ranging from 38.93% in *Ficus langkokensis* to 54.66% in *Macropanax dispermus* (Table 1). This significant intraspecific variability highlighted the diversity of metabolites within species.

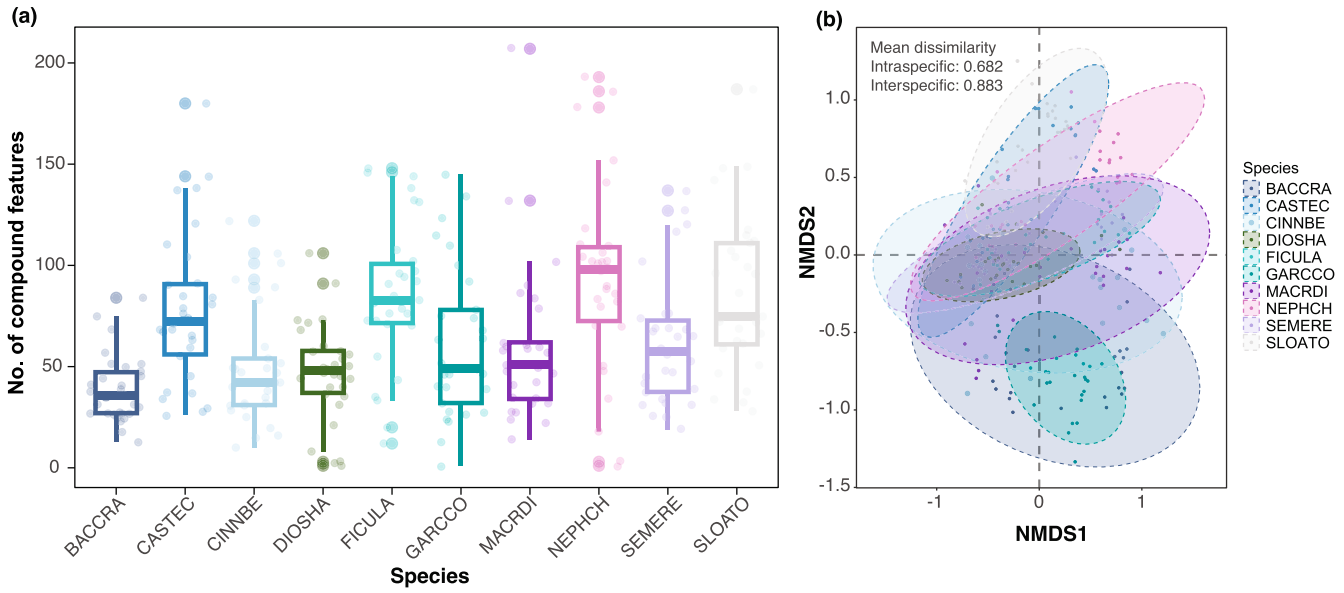

Fig. 1 Foliar metabolite profiles of 300 individuals. (a) Boxplot of metabolite richness of 10 species. (b) NMDS visualization based on dissimilarity matrix for all metabolites across 10 species. The boxplots display the interquartile range (IQR; 25th–75th percentiles) as boxes, with a central horizontal line marking the median. Whiskers extend to 1.5 times the IQR from the box edges; individual observations are shown as small circles, and larger circles highlight potential outliers (values beyond 1.5 × IQR). Permutational analysis of variance (PERMANOVA) tests indicate species identity had a significant effect on dissimilarity among individuals ($P = 0.001$). Species code: BACCRA, *Baccaurea ramiflora*; CASTEC, *Castanopsis echinocarpa*; CINNBE, *Cinnamomum bejolghota*; DIOSHA, *Diospyros hasseltii*; FICULA, *Ficus langkokensis*; GARCCO, *Garcinia cowa*; MACRDI, *Macropanax dispermus*; NEPHCH, *Nephelium chryseum*; SEMERE, *Semecarpus reticulatus*; SLOATO, *Sloanea tomentosa*.

Table 1 Statistical summary and Kvålseth's coefficient of variation (^{K}CV) of compound richness across the 10 species.

Species	Family	Max	Min	Mean	SD	^{K}CV (%)
Ficus langkokensis Drake	Moraceae	148	12	86	36	38.93
Baccaurea ramiflora Lour.	Euphorbiaceae	84	13	39	17	39.41
Sloanea tomentosa (Benth.) Rehder & E. H. Wilson	Elaeocarpaceae	187	28	87	39	41.11
Castanopsis echinocarpa A. DC.	Fagaceae	180	26	78	38	43.53
Nephelium chryseum Blume	Sapindaceae	193	1	93	47	45.07
Semecarpus reticulatus Lecomte	Anacardiaceae	137	19	62	32	45.55
Diospyros hasseltii Zoll.	Ebenaceae	106	1	47	24	46.12
Cinnamomum bejolghota (Buch.-Ham.) Sweet	Lauraceae	122	10	50	29	50.42
Garcinia cowa Roxb.	Guttiferae	145	1	61	38	52.60
Macropanax dispermus (Blume) Kuntze	Araliaceae	207	14	59	39	54.66

Following the NMDS analysis, we observed that each species occupies a large chemical space due to substantial intraspecific variation, resulting in some overlap between species (Fig. 1b). However, despite this visual overlap, permutational ANOVA revealed significant interspecific differences in the overall chemical space as well as across seven biosynthetic pathways, indicating that each species maintains distinct chemical characteristics (Fig. S3; Table S3). We further examined the compound composition across species by analyzing the proportion of compounds in various biosynthetic pathways, revealing differences among species (Fig. 2a). For instance, in *Baccaurea ramiflora*, fatty acids were more abundant than terpenoids, whereas in *Garcinia cowa*, the reverse was observed. We also assessed the degree of metabolite variation by comparing mean dissimilarity within and between species across different compound categories, including total, primary, and secondary metabolites, as well as seven major biosynthetic pathways (Fig. S4). For total metabolites, the mean intraspecific dissimilarity was 0.682, while the mean interspecific dissimilarity was 0.883. Similar to total metabolites, the mean interspecific dissimilarity was higher than the mean intraspecific dissimilarity for each of the seven major biosynthetic pathways (Fig. S4). However, the substantial intraspecific variation observed in metabolite profiles is noteworthy, as it is often comparable to, and in some cases nearly as high as, the interspecific variation, underscoring the significant role of intraspecific variability.

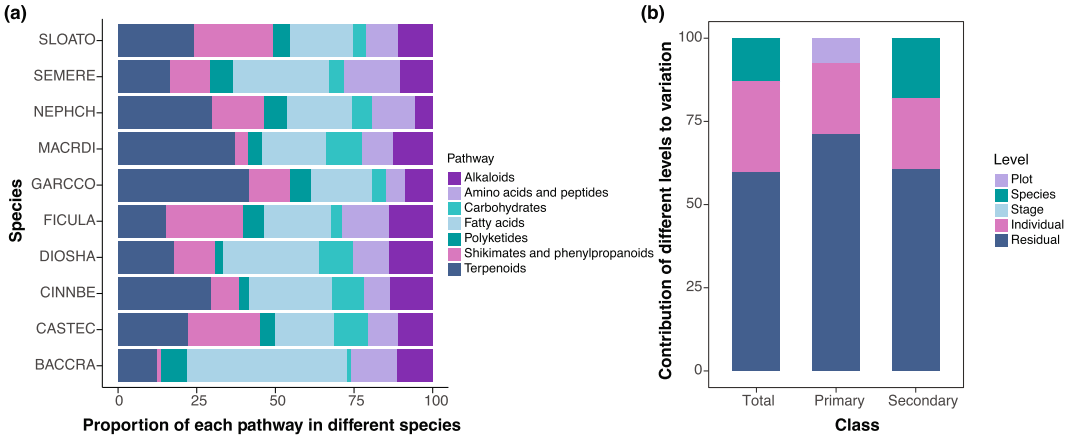

Fig. 2 Hierarchical variance decomposition of foliar metabolites. (a) Composition of foliar metabolites across 10 common species. (b) Contributions of four hierarchical levels to variation in total, primary, and secondary metabolites. Species code: BACCRA, *Baccaurea ramiflora*; CASTEC, *Castanopsis echinocarpa*; CINNBE, *Cinnamomum bejolghota*; DIOSHA, *Diospyros hasseltii*; FICULA, *Ficus langkokensis*; GARCCO, *Garcinia cowa*; MACRDI, *Macropanax dispermus*; NEPHCH, *Nephelium chryseum*; SEMERE, *Semecarpus reticulatus*; SLOATO, *Sloanea tomentosa*.

Sources of variation in foliar metabolites

Our nested variance decomposition analysis indicated that the largest proportion of variation in total foliar metabolites was among individuals, contributing 27.5% of the total variance (Fig. 2b). Variation among species contributed 12.88%, making it the second-largest source of variation (Fig. 2b). By contrast, 'life stage' and 'plot' contributed minimally, suggesting these factors had little consistent influence on the variation in foliar metabolites. When the analysis was further partitioned into primary and secondary metabolites, distinct patterns of contribution emerged (Fig. 2b). For primary metabolites, plot-level factors explained 7.65% of the variation, while the contribution of individual-level differences remained substantial at 21.41%. Notably, 'species' showed negligible contributions to primary metabolite variation. By contrast, for secondary metabolites, species-level contributions became more pronounced, explaining 18% of the total variance, while individual-level differences remained similar at 21.5%.

Relative importance of genetic diversity, abiotic environment, and biotic environment

Our results (Figs 3, 4) illustrate the contributions of genetic diversity, abiotic environment, biotic environment, and their interactions to intraspecific variation across different metabolite categories, including total, primary, and secondary metabolites as well as seven major biosynthetic pathways. By comparing R^2 values and significance levels for each model (Figs S5, S6), we observed distinct responses of intraspecific variation to genetic, abiotic, and biotic factors among species, which enabled us to determine whether compounds within the same category consistently respond to specific factors across species or whether substantial interspecies variability exists.

For total metabolites (Fig. 3a), the largest contributor to intraspecific variation was the biotic environment. For example, in *Diospyros hasseltii*, the most significant factor influencing intraspecific variation was the biotic environment, along with the interaction between genetic diversity and the biotic environment (Figs 3a, S5a). Moreover, the responses of intraspecific variation in total metabolites to biotic factors displayed greater interspecies variability than responses to abiotic or genetic factors (Fig. 3a). This variation suggests that biotic factors exert diverse influences across species, indicating distinct adaptive strategies in metabolite profiles among species.

For primary metabolites (Fig. 3b), genetic, abiotic, and biotic factors had relatively balanced contributions to intraspecific variation, with responses showing less interspecies variability. However, within specific pathways such as 'Carbohydrates' (Fig. 4f), abiotic factors were the dominant contributors. For instance, in *Macropanax dispermus*, the abiotic environment was the primary factor affecting intraspecific variation in carbohydrates (Figs 4f, S6f). Notably, responses of carbohydrate variation to abiotic factors were more divergent among species than those to genetic or biotic factors (Fig. 4f).

For secondary metabolites (Fig. 3c), the pattern of intraspecific variation was similar to that of total metabolites, with biotic factors having a predominant influence. For example, in *Macropanax dispermus*, intraspecific variation in 'Amino Acids and Peptides' (Figs 4b, S6b) was primarily influenced by biotic factors, while in *Garcinia cowa*, biotic factors had the largest impact on intraspecific variation in 'Terpenoids' (Figs 4e, S6e). In particular, the magnitude of intraspecific variation in responses to biotic factors differed considerably among species within pathways such as 'Alkaloids' (Fig. 4a), 'Amino Acids and Peptides' (Fig. 4b), and 'Polyketides' (Fig. 4c), suggesting that species exhibit distinct responses to biotic interactions.

While abiotic and biotic factors emerged as important influences on intraspecific variation across different metabolite categories, our analysis also highlighted the substantial role of genetic background and its interactions with environmental factors (Figs 3, 4). Across all metabolite categories, interactions between

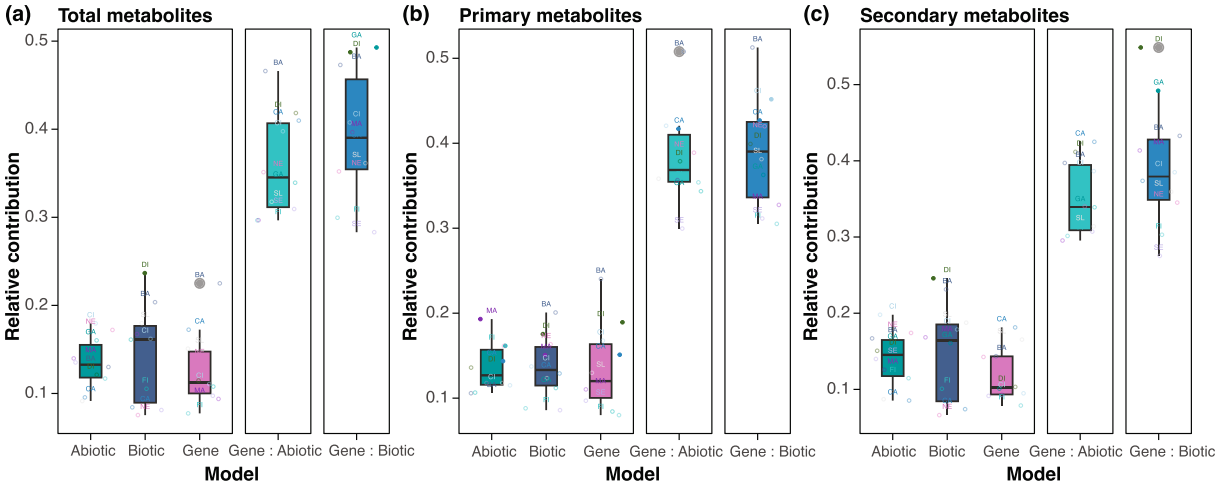

Fig. 3 Contributions of genetic, abiotic, and biotic factors to intraspecific dissimilarity in total, primary, and secondary metabolites. Boxplots show the relative contributions of genetic diversity, abiotic environment, and biotic environment to intraspecific dissimilarity across 10 plant species, with subplots representing (a) total metabolites, (b) primary metabolites, and (c) secondary metabolites, analyzed via R^2 values. Points represent individual species, with closed points indicating significant effects ($P < 0.05$) and open points indicating nonsignificant effects ($P \geq 0.05$). Contributions were assessed using three models: (1) individual effects; (2) gene–abiotic interactions; and (3) gene–biotic interactions. Model significance was determined via 999 permutation tests. The boxplots display the interquartile range (IQR; 25th–75th percentiles) as boxes, with a central horizontal line marking the median. Whiskers extend to 1.5 times the IQR from the box edges, individual observations are shown as small circles, and larger circles highlight potential outliers (values beyond 1.5 × IQR). Species code: BA, *Baccaurea ramiflora*; CA, *Castanopsis echinocarpa*; CI, *Cinnamomum bejolghota*; DI, *Diospyros hasseltii*; FI, *Ficus langkokensis*; GA, *Garcinia cowa*; MA, *Macropanax dispermus*; NE, *Nephelium chryseum*; SE, *Semecarpus reticulatus*; SL, *Sloanea tomentosa*.

genetic diversity and abiotic or biotic environments showed high R^2 values, indicating a significant impact on intraspecific variation. This finding underscores the importance of considering genetic–environment interactions when examining factors that influence metabolite diversity within species.

Discussion

The plant metabolome mediates interactions with natural enemies, mutualists, and the abiotic environment, influencing resource allocation trade-offs that shape life-history strategies and defense syndromes (Coley *et al.*, 1985; Kursar & Coley, 2003). However, plant metabolites exhibit substantial intraspecific variation driven by genetic and environmental factors (Glassmire *et al.*, 2016; Salgado *et al.*, 2023). This study assessed intraspecific metabolite variation, its role in community-level metabolite diversity, and the genetic and environmental contributions to this variation in co-occurring tree species in a seasonal tropical forest. We found that individual-level variation was the largest source of metabolite diversity, followed by species-level variation (Fig. 2b). The metabolic pathways linked to genetic and environmental variation differed among species (Fig. 4). Our results highlight intraspecific variation as a key driver of community metabolite diversity. However, species rely on different metabolite classes to cope with environmental pressures, underscoring the role of genetic variation and plasticity. Furthermore, interspecific variation shapes the relative influence of these drivers within species, as well as the predominant biosynthetic pathways that they affect.

Importance of intraspecific metabolite variation in tree communities

Intraspecific trait variation is increasingly recognized as ecologically significant across morphological (Hulshof & Swenson, 2010) and physiological traits (Martin *et al.*, 2017). Community-level studies reveal that morphological ITV is comparable to interspecific variation, accounting for 25% of within-community and 32% of between-community trait differences (Messier *et al.*, 2010; Siefert *et al.*, 2015). These levels suggest that predictions of ecological dynamics based on species mean trait values may be flawed (Yang *et al.*, 2018; Rubio & Swenson, 2024). Despite these insights, research on ITV remains disproportionately focused on easily measurable phenotypic traits, and most studies that have explored metabolomic variation in the context of functional ecology have done so using species mean trait values (Sardans *et al.*, 2011; Endara *et al.*, 2022; Walker *et al.*, 2022).

Our findings demonstrate substantial intraspecific variation in foliar metabolomes, with individual-level differences explaining 27.5% of total variance—consistent with population-specific metabolite diversity in *Cistus ladanifer* (Masa *et al.*, 2016) and global herbivory variation patterns (Robinson *et al.*, 2023). On the other hand, interspecific chemical dissimilarity (mean = 0.883) clearly exceeds intraspecific levels (mean = 0.682). This apparent discrepancy can be reconciled. Mean dissimilarity quantifies compositional divergence between species, whereas variance decomposition assesses hierarchical contributions. Furthermore, our results suggest that species possess distinct metabolic toolkits, and in many cases unique metabolites, yet individuals vary as to

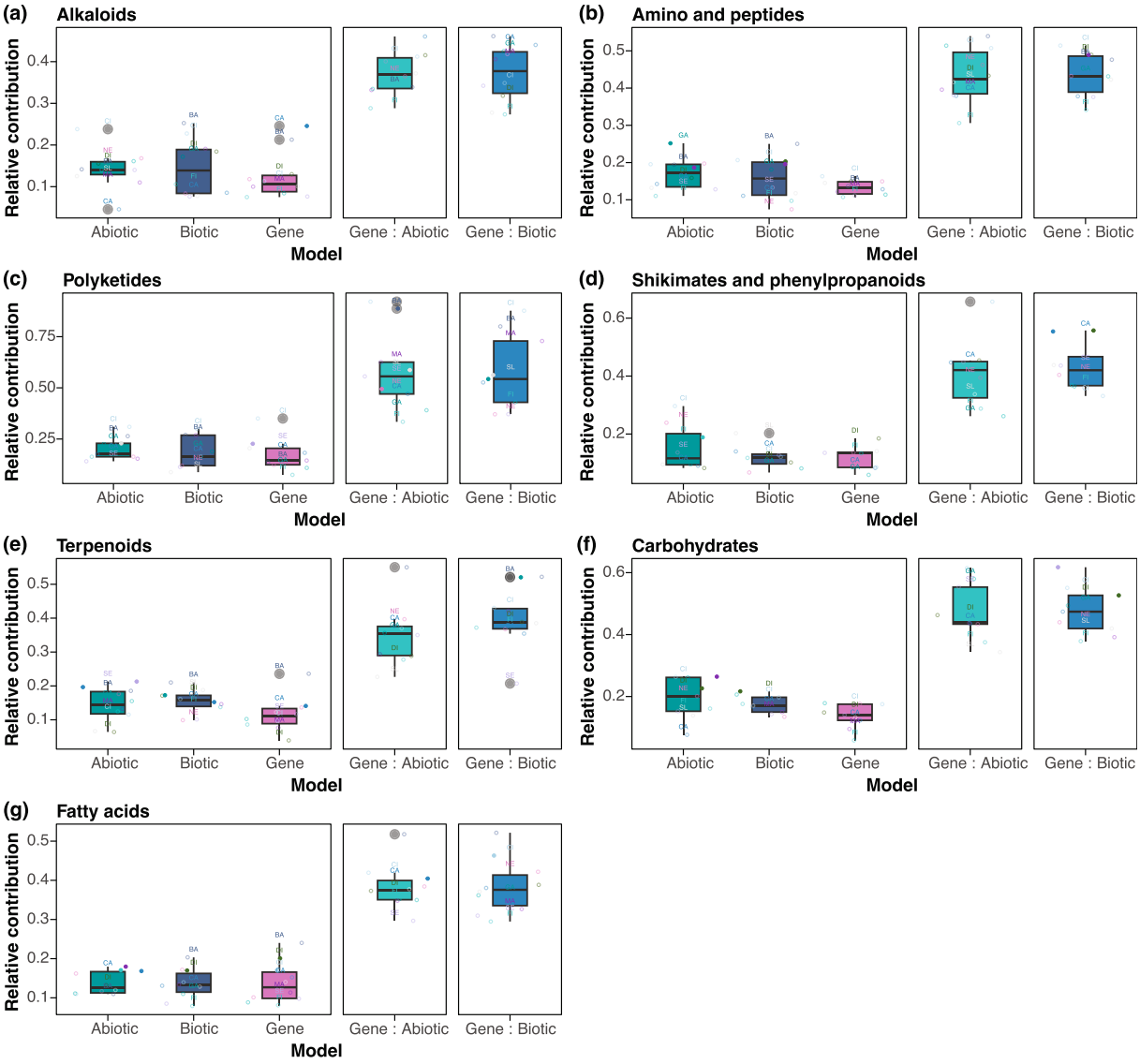

Fig. 4 Contributions of genetic, abiotic, and biotic factors to intraspecific dissimilarity across seven major biosynthetic pathways. Boxplots show the relative contributions of genetic diversity, abiotic environment, and biotic environment to intraspecific dissimilarity across seven major biosynthetic pathways (a–g) of 10 species, based on R^2 values. Points represent individual species, with closed points indicating significant effects ($P < 0.05$) and open points indicating nonsignificant effects ($P \geq 0.05$). Contributions were assessed using three models: (1) individual effects; (2) gene–abiotic interactions; and (3) gene–biotic interactions. Model significance was determined via 999 permutation tests. The boxplots display the interquartile range (IQR; 25th–75th percentiles) as boxes, with a central horizontal line marking the median. Whiskers extend to 1.5 times the IQR from the box edges, individual observations are shown as small circles, and larger circles highlight potential outliers (values beyond 1.5 × IQR). Species code: BA, *Baccaurea ramiflora*; CA, *Castanopsis echinocarpa*; CI, *Cinnamomum bejolghota*; DI, *Diospyros hasseltii*; FI, *Ficus langkokensis*; GA, *Garcinia cowa*; MA, *Macropanax dispermus*; NE, *Nephelium chryseum*; SE, *Semecarpus reticulatus*; SL, *Sloanea tomentosa*.

which metabolites are expressed. As a result, individual-to-individual differences make up a significant proportion of community-scale chemical variation, with the potential to reshape our understanding of plant adaptation and ecosystem functioning.

In tropical forests, the role of biotic interactions is important to understanding potential mechanisms of coexistence among species. Negative intraspecific interactions must be stronger than negative interspecific interactions for species to stably coexist (Adler *et al.*, 2018), and this niche differentiation can be achieved by species divergence in traits that mediate resource use or interactions with natural enemies (Chesson & Kuang, 2008). While opportunities for differentiation in plants with respect to resources are few, insect herbivores and microbial pathogens represent a high-dimensional space within which plants might differentiate to avoid enemy-mediated competition. Janzen (1970) and Connell (1971) proposed that, as a result of plant differentiation with respect to host range-limiting traits such as chemical defenses, specialist natural enemies may suppress their host plants where locally abundant. This dynamic enforces

intense, enemy-mediated competition, thereby promoting species coexistence. The diversity of density-dependent enemies can likely vary with the degree of chemical divergence among plants and hence overlap in natural enemies (Sedio & Ostling, 2013). Empirical studies of *Inga* (Fabaceae) based on species average metabolomes found that chemical similarity is associated with the degree to which herbivores are shared among species (Kursar *et al.*, 2009; Endara *et al.*, 2017) and that chemical similarity to neighbors reduces sapling survival (Forrister *et al.*, 2019). Furthermore, local neighborhoods consist of species that are less chemically similar than random in the Xishuangbanna, China, forest dynamics plot, our study site (Wang *et al.*, 2023; Sun *et al.*, 2024). Yet other studies have found that variation in the chemical profiles of individual plants can affect their palatability and susceptibility to herbivores (Massad *et al.*, 2011; Glassmire *et al.*, 2016). Hence, our findings suggest that considering intraspecific variation in metabolomes will provide valuable insights into resource utilization, competition, and diversity maintenance, even in species-rich tropical forests.

The contribution of the abiotic and biotic environment to intraspecific variation in plant metabolites

Our findings support a growing body of evidence that different metabolite classes respond differentially to abiotic and biotic environmental variation (Fig. 4; Table S4; Volf *et al.*, 2023). In our study, primary and secondary metabolites exhibited distinct responses to these factors, with primary metabolites more strongly influenced by abiotic conditions and secondary metabolites showing a greater response to biotic interactions (Fig. 3b,c). We defined primary metabolites as carbohydrates and fatty acids to distinguish them from more specialized metabolic pathways that are more likely to be involved in defense. Variations in carbohydrates and fatty acids may reflect underlying plant physiology and adaptations to abiotic environmental stresses such as drought, temperature fluctuations, and nutrient availability (Sampaio *et al.*, 2016; Das *et al.*, 2017; Salam *et al.*, 2023). Furthermore, abiotic stress can significantly alter the expression of metabolic pathways associated with primary metabolites, resulting in changes in plant growth and survival strategies (Abd El-daim *et al.*, 2019; Godoy *et al.*, 2021).

By contrast, secondary metabolites encompass a vast diversity of plant compounds with numerous and sometimes multiple functions, including responses to abiotic stress and defense against herbivores and pathogens (Volf *et al.*, 2023). Their production is often induced by herbivory or pathogen attack (Jan *et al.*, 2021; Al-Khayri *et al.*, 2023). For example, research has demonstrated that the accumulation of secondary metabolites such as alkaloids and phenolics is significantly influenced by biotic stressors, which induce their biosynthesis (Ghorbanpour *et al.*, 2013; Erb & Kliebenstein, 2020). In addition to induction in direct response to the attack by natural enemies, environmental factors such as soil composition and moisture levels can modulate biotic interactions, further shaping the relationship between secondary metabolite production and environmental conditions (Erb & Lu, 2013; Walter, 2018; Bennett & Klironomos, 2019). The growth–differentiation balance hypothesis provides a valuable framework for understanding trade-offs in investment between growth and defense faced by individuals (Herms & Mattson, 1992). According to this hypothesis, individuals respond to favorable resource conditions (e.g. high soil nutrient availability) by investing in primary metabolism and growth, whereas individuals that experience resource limitation invest in secondary metabolites for defense. Recent studies have found that both biotic (e.g. competition and herbivory) and abiotic (e.g. nutrient availability) factors shape metabolome expression (Ballaré & Austin, 2019; Volf *et al.*, 2022). Hence, variations in soil nutrients, crowding, and herbivory all likely contributed to intraspecific metabolite variation across our 10 focal species.

Although most species exhibited some variation in response to the abiotic or biotic environment or their interaction with genetic distance (Figs 4, S6), our results suggest that the particular metabolic pathways that respond to such variation vary among species. For example, in *Castanopsis echinocarpa*, abiotic and biotic factors significantly affected intraspecific variation in shikimates, terpenoids, and fatty acids (Figs 4d,e,g, S6d,e,g), suggesting that these metabolites play an important role in defense and/or stress response (Huber *et al.*, 2016). By contrast, in *Baccaurea ramiflora*, variation in the abiotic and biotic environment was associated with intraspecific variation in polyketides (Figs 4c, S6c), suggesting a reliance on a distinct metabolic pathway for defense. Polyketides are known for their diverse biological activities, including antimicrobial properties, which can be crucial for plants facing varying environmental stresses (Volf *et al.*, 2022). These species-specific metabolic responses likely reflect metabolic pathways that are unique to specific plant phylogenetic lineages, well-known examples of which include glucosinolates in Brassicaceae and quinolizidine alkaloids in Fabaceae (Wink, 2003). Such lineage-characteristic biosynthetic pathways may have evolved in response to different selection pressures experienced by different lineages during their evolutionary history. Hence, the variation in metabolic pathways we observed among species likely reflects a deep phylogenetic signal that distinguishes the families represented by our 10 focal species (Wink, 2003). Such lineage-specific metabolic strategies may contribute to niche differentiation by allowing species to mitigate competition through distinct resource allocation patterns. However, a growing body of evidence suggests that even closely related tree species often display distinctive and characteristic metabolomic composition perhaps especially in species-rich tropical tree genera (Sedio *et al.*, 2017; Endara *et al.*, 2018). Although this is often seen as evidence for within-site niche partitioning with respect to defensive metabolites (Kursar *et al.*, 2009; Forrister *et al.*, 2019), interspecific metabolomic variation may also contribute to abiotic niche segregation among closely related species despite ITV (Volf *et al.*, 2022, 2023). As a consequence of the fundamental differences in metabolic pathways that co-occurring species rely on for similar functions, interspecific variation represents an important component of metabolite diversity at the scale of the forest community. This holds true even when considering the magnitude of intraspecific variation we observed.

The contribution of genetic diversity to intraspecific variation of plant metabolites

Understanding the role of genetic diversity in intraspecific metabolite variations is crucial for elucidating plant adaptation to environmental changes. Genetic diversity can enhance a population's ability to adapt to varying environmental conditions, which is essential for survival and reproduction in fluctuating ecosystems (Crawford & Whitney, 2010). Previous research has shown that genetic variation can lead to significant differences in chemical profiles, influencing traits such as herbivore resistance and disease tolerance (Pardo *et al.*, 2018). For instance, studies have demonstrated that even minor genetic differences, such as single amino acid substitutions, can result in substantial variation in secondary metabolite production, which, in turn, can affect plant fitness and interactions with herbivores (Pais *et al.*, 2018). In our study, we found that genetic factors exerted a less significant influence on intraspecific metabolite variation compared to environmental factors. Specifically, we observed that genetic distance primarily affected intraspecific variation in fatty acids (Figs 4g, S6g), which we defined as primary metabolites, as well as certain secondary metabolites such as alkaloids and terpenoids (Figs 4a,e, S6a,e). This pattern aligns with our expectations and can be attributed to several factors.

First, our community-level sampling revealed limited genetic diversity, likely due to the relatively small spatial extent (20 ha) of the sampled community. This limited genetic diversity may restrict the range of metabolic responses available to individuals within the population (Riedelsheimer *et al.*, 2012). Moreover, the dynamics of plant metabolite production are often rapid and responsive to environmental changes (Metlen *et al.*, 2009; Moore *et al.*, 2014), which can overshadow heritable variation due to genetics. As environmental conditions fluctuate, plant individuals may quickly adjust their metabolite profiles to optimize growth and defense strategies. This rapid response diminishes the observed association between genotype and phenotype in the population.

However, the interplay between genetic diversity and environmental conditions creates a dynamic landscape of metabolite expression, in which both abiotic and biotic influences converge to shape the chemical ecology of a species. For example, studies have shown that genetic diversity can enhance the resilience of plant populations to environmental stressors, thereby influencing the production of secondary metabolites that function in defense against herbivores and pathogens (Isah, 2019; Jan *et al.*, 2021). This suggests that, while genetic diversity may play a crucial role in underpinning potential adaptation to environmental changes, its contribution to observed phenotypic variation within a population is difficult to detect in the face of the extreme phenotypic plasticity and dynamic variation in expression exhibited by plant metabolites. Moreover, variation in natural selection pressures, which shape responses in growth and defense traits based on their impact on plant fitness, adds another layer of complexity to this relationship. Future work should further compare the relative importance of genetic and abiotic/biotic environmental factors and their interactions in shaping intra- and interspecific variation in plant metabolites across a range of spatial and temporal scales in multiple forest types.

Conclusion

Our study highlights the crucial role of intraspecific metabolite variation in shaping community-level chemical diversity in tropical forests. We demonstrate that while species differ in the metabolic pathways and chemical classes they express to cope with ecological pressures, both genetic diversity and environmental factors exert significant influence on the metabolite profiles of individual trees. By integrating metabolomics with genetic and environmental analyses, our study provides novel insights into the ecological and evolutionary mechanisms underlying plant chemical diversity. These findings suggest that both metabolic plasticity and genetic variation make significant contributions to community-level chemical variation and raise important questions about the implications of this variation for interspecific competition and diversity maintenance. Future research should explore how these sources of metabolomic variation respond to broader environmental gradients and how such variation influences higher trophic interactions and long-term community dynamics in tropical ecosystems.

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Competing interests

None declared.

Author contributions

JY, JRL, MC and NGS designed the study. YH and GX carried out the experiments. YH and MA collected and processed the samples. YH, JX, RRJ and BES analyzed the data with input from all authors. YH, NGS, JY and BES wrote the manuscript.

YH, JY and GX revised the manuscript. All authors provided feedback on the manuscript.

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Data availability

The data that support the findings of this study are openly available in the Science Data Bank at doi: 10.57760/sciencedb.22062, reference number 22062.

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Supporting Information

Additional Supporting Information may be found online in the Supporting Information section at the end of the article.

Fig. S1 Geographical location of the 20-ha Xishuangbanna forest dynamics plot.

Fig. S2 The relative proportions of the seven biosynthetic pathway compounds in 10 species.

Fig. S3 Nonmetric multidimensional scale visualization of compounds for 10 species.

Fig. S4 Comparison of intra- and interspecific mean dissimilarity.

Fig. S5 Contributions of genetic, abiotic, and biotic factors to intraspecific dissimilarity in total, primary, and secondary metabolites.

Fig. S6 Contributions of genetic, abiotic, and biotic factors to intraspecific dissimilarity across seven major biosynthetic pathways.

Methods S1 Next-generation sequencing.

Methods S2 Genetic data processing.

Methods S3 Metabolite annotation.

Table S1 Abundances of 10 focal species in the 20-ha Xishuangbanna forest dynamics plot.

Table S2 Loading of abiotic variables on three principal components of variation.

Table S3 Results of PERMANOVA of interspecific variation in CSCS among 10 species.

Table S4 Results of PERMANOVA assessing genetic, abiotic, and biotic influences on metabolite variation at the community level.

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