

Human-mediated community assembly reshapes urban phytochemical diversity

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Abstract

Human activities increasingly determine which plant species coexist, particularly in cities, yet whether this reshapes the chemical dimension of biodiversity remains largely unknown. Here, we investigated how human-mediated plant community assembly influences phytochemical diversity by integrating community composition, functional traits, phylogenetic relationships, leaf metabolomes, and floral volatile profiles across 60 urban green spaces spanning a wide gradient of human influence in Zurich, Switzerland. Human influence was associated with greater phytochemical richness, an effect mediated primarily through increases in plant functional diversity. Human influence was also associated with coordinated shifts in functional, phylogenetic, and phytochemical composition, generating distinct chemical assemblages across urban green space types. Yet phytochemical differentiation was especially sensitive to fine-scale species turnover: chemically distinct communities emerged even when species replacement produced relatively little divergence in broader functional or phylogenetic structure. These patterns were strikingly consistent between leaf metabolites and floral volatiles despite their contrasting ecological functions and evolutionary constraints. Our findings reveal phytochemical diversity as an emergent property of community assembly and show that human decisions can reorganize the chemical environments through which ecological interactions occur.

Main

Humans increasingly determine which species coexist, particularly in cities, where plant communities are shaped not only by environmental filtering but also by deliberate decisions about which species to plant, maintain, or remove^{1,2}. Urban green spaces (UGS) therefore provide a powerful setting in which to examine how human decisions alter community assembly. These spaces are increasingly important for supporting biodiversity, ecosystem functioning and human well-being as cities and urban populations grow^{3–6}. Yet, urban vegetation is still predominantly designed according to human preferences rather than ecological principles⁷. The consequences of such decisions are typically evaluated through visible changes in vegetation structures, species richness, and community composition (e.g.,⁸). Whether human-mediated assembly also reshapes less visible dimensions of biodiversity, however, remains largely unknown.

One such dimension is plant chemistry. Plants produce extraordinarily diverse mixtures of metabolites that mediate interactions with herbivores, pollinators, pathogens, and other organisms, thereby contributing to ecosystem processes and services^{9,10}. At the community level, the identities of co-occurring plant species therefore determine the chemical environment experienced by interacting organisms: Leaf-associated metabolites mostly mediate plant-herbivore interaction, whereas floral volatiles shape communication with pollinators through attraction and signaling^{10–12}. Because plant chemistry is partly structured by evolutionary history, turnover in plant community composition can translate into changes in community-level phytochemical composition^{13–15}. Yet these evolutionary constraints can differ among plant organs and chemical functions¹⁶. In particular, evidence suggests that leaf metabolomes can retain substantial phylogenetic structure^{17,18}, whereas floral volatiles may evolve more rapidly under selection associated with pollinator attraction and reproduction^{11,19}. Human-driven community assembly may therefore reorganize

different components of the urban phytochemical landscape in distinct, and potentially difficult to predict, ways, with cascading consequences for herbivory, pollination, and ecosystem functioning^{10–12}.

Plant selection in cities is rarely guided by chemical traits or evolutionary history²⁰. Instead, species are often chosen according to visible characteristics, perceived utility, and cultural or aesthetic preferences^{21,22}. Subjective selection for such attributes can alter both the functional and phylogenetic structure of urban floras (Fig. 1), with the strength and direction of this filtering varying among urban green-space types^{2,8,23}; ruderal areas, for instance, are shaped mainly by environmental conditions and spontaneous colonization, whereas parks, gardens, and allotments are subject to progressively stronger influences of deliberate species selection, often including non-native taxa chosen for food production or ornamental value^{8,24,25}. Such contrasts provide a gradient of human-mediated community assembly through which functional, phylogenetic and chemical dimensions of biodiversity may become reorganized (Fig. 1). However, we do not know whether these dimensions change in concert, whether phytochemical differentiation simply reflects taxonomic, functional and phylogenetic turnover, or whether chemically distinct communities can emerge even from relatively subtle replacement among functionally or evolutionarily similar species.

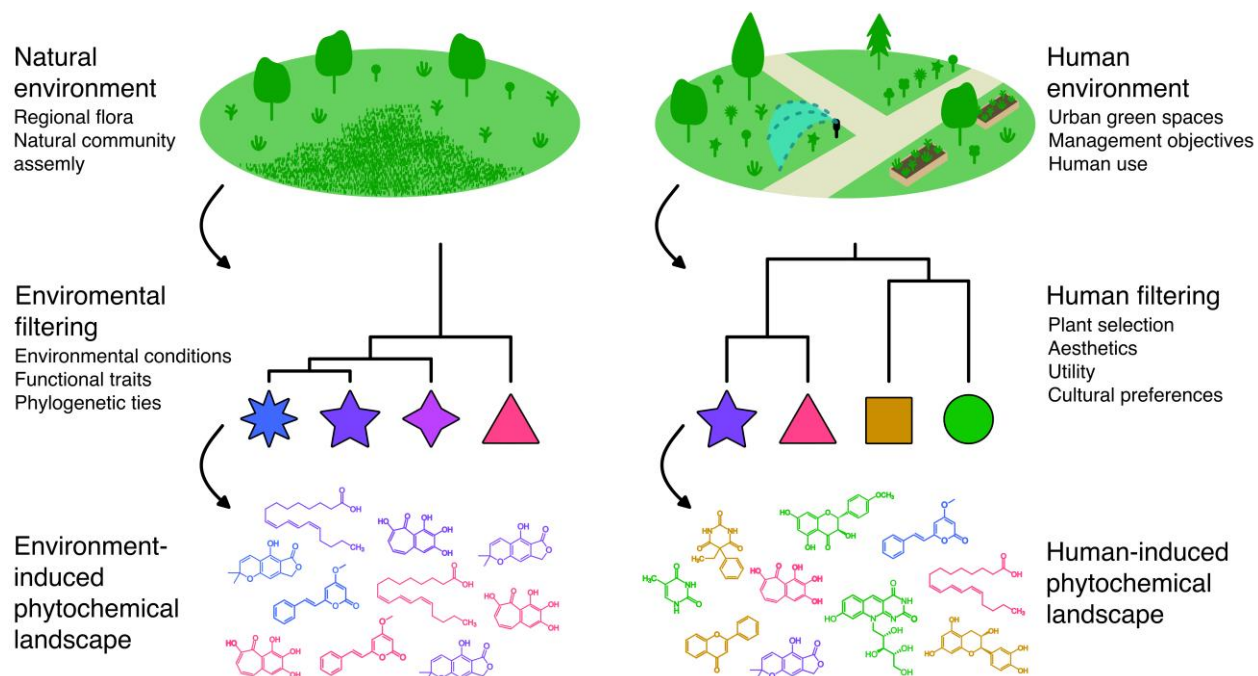


Figure 1. Conceptual framework illustrating how ecological and anthropogenic filters shape urban phytochemical landscapes. In natural environments, ecological filtering assembles plant communities from the regional species pool based on species traits, generating phytochemical landscapes modulated by evolutionary ties among species. In urban green spaces, environmental modification and plant selection based on human preferences restructure community composition, potentially altering the diversity and composition of leaf- and flower-associated metabolites. Colors and shapes represent species and their traits, with greater similarity indicating greater similarity in traits and evolutionary relatedness.

Here, we investigated how human-mediated plant community assembly restructures urban phytochemical landscapes by integrating plant community composition, functional traits, phylogenetic relationships, leaf metabolomes, and floral volatile profiles across 60 urban green spaces in Zurich, Switzerland. We surveyed 539 vascular plant species across five UGS types that differ in intended function, management intensity, and vegetation assembly: ruderal areas, parks, residential areas owned by real-estate companies (henceforth, “real-estate areas”), private gardens, and allotments. These green spaces capture a gradient of vegetation assembly, from spontaneously

88 assembled, low-management communities dominated by stress-tolerant species in ruderal areas, to
89 intensively managed communities shaped by intentional planting decisions in allotments, with
90 parks, real-estate areas and private gardens representing intermediate forms of human selection and
91 management. We asked whether (1) increasing human influence is associated with coordinated
92 shifts in functional, phylogenetic and phytochemical composition, (2) chemical turnover can
93 emerge independently of broad functional and phylogenetic divergence, and (3) human influence
94 alters phytochemical diversity directly or indirectly through changes in functional and phylogenetic
95 diversity. We further assessed whether these relationships differ between leaf metabolites and floral
96 volatiles, given their contrasting ecological and evolutionary constraints. By treating
97 phytochemical diversity as an emergent property of community assembly, our study examines how
98 human decisions reshape the largely hidden chemical landscapes through which species interact.

100 **Results**

101 Across the 60 study sites, we characterized plant community composition through standardized
102 transect surveys conducted across three sampling periods spanning the 2024 growing season and
103 compiled functional trait information for all 539 vascular plant species (see ^{26,27}). Species-level
104 trait data included 26 functional traits representing two complementary dimensions of urban plant
105 assembly: human-associated traits linked to plant selection and management decisions (e.g., growth
106 form, floral characteristics, leaf morphology and species origin), and broader ecological traits
107 related to environmental preferences, physiology and life-history strategies (Table S1). We further
108 reconstructed species-level phylogenetic relationships and quantified variation in human influence
109 among urban green spaces using a management-based index derived from a validated 42-item
110 questionnaire completed by local managers (see ^{25,28}). This index (henceforth, “human influence

index”) integrates manager time investment as a proxy for ecological stewardship ²⁹, with higher values indicating greater time and effort devoted to green space management.

We then generated complementary metabolomic datasets for leaves and flowers. Untargeted metabolomics detected 18,972 leaf-associated metabolite features across 416 species and 1,822 flower-associated metabolites across 380 species, with 257 species characterized for both organs. Despite their contrasting ecological roles and analytical platforms, leaf and floral chemical richness were weakly but significantly correlated across the shared species (Spearman's $r = 0.25$, $P < 0.001$). We reconstructed community-level phytochemical composition by combining the metabolite profiles of all species occurring within each community, enabling comparisons with taxonomic, functional and phylogenetic community structure (Fig. S1). Using these complementary dimensions of biodiversity, we assessed whether and at what ecological scales human influence reorganizes chemical composition alongside functional and phylogenetic diversity, identified the human-associated and ecological traits associated with these shifts, and quantified the pathways linking human influence to phytochemical richness.

Human-mediated community assembly creates distinct phytochemical signatures

To test whether human-mediated community assembly generated coordinated changes in phytochemical, functional, and phylogenetic composition, we compared chemical, functional, and phylogenetic community composition using principal coordinate analyses (PCoA) and quantified their concordance through Procrustes superimposition of the resulting ordinations. We found that human influence structured plant communities across chemical, functional, and phylogenetic dimensions (Fig. 2). Procrustes analyses revealed significant concordance among these ecological spaces for both leaf- and flower-associated metabolites, indicating parallel shifts in community composition across chemical, functional, and phylogenetic dimensions (Fig. 2; Fig. S2).

Community composition was further organized along the human-influence gradient, with clear separation among UGS types. Allotments, ruderal areas, and parks occupied distinct regions of ordination space, whereas private gardens and real-estate areas were intermediate. Chemical richness also differed among UGS types, following the same ranking as plant species richness (Fig. S3), with highest richness in allotments and lowest in ruderal areas (Fig. S4).

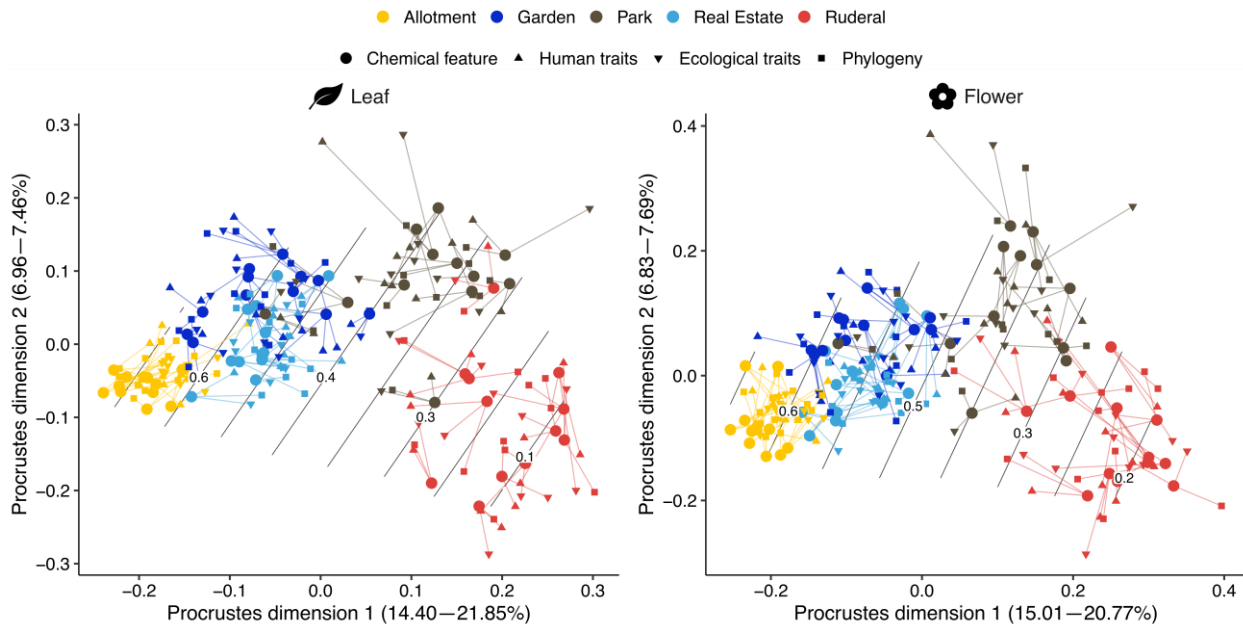


Figure 2. Procrustes superimposition of trait, phylogenetic, and metabolomic feature compositions for leaf (left) and flower (right) communities across urban green space types (color-coded). Large circles represent the reference chemical feature configuration, while smaller symbols indicate the aligned positions after Procrustes rotation for human-associated traits (triangles), broader ecological traits (squares), and phylogeny (circles). Line segments connect matched points between ordinations, with shorter segments indicating greater concordance among data spaces. Grey contour lines show the generalized additive model (GAM)-fitted surface of the human-influence index across chemical feature space. Values shown for each axis indicate the range of variance explained by the first and second dimensions of the chemical, functional, and phylogenetic composition spaces independently.

150 To determine the ecological scales at which community assembly predicts phytochemical
151 differentiation, we related pairwise chemical dissimilarities among sites to complementary
152 measures of functional and phylogenetic turnover. Specifically, we compared chemical
153 composition against mean pairwise distance (MPD), reflecting turnover among broader functional
154 or evolutionary groups, and mean nearest taxon distance (MNTD), capturing finer-scale
155 replacement among functionally or phylogenetically similar species. This approach revealed that
156 the relationship between community dissimilarity and chemical turnover depended on the scale of
157 ecological differentiation (Fig. 3): across communities, fine-scale functional and phylogenetic
158 turnover (MNTD) explained chemical dissimilarity more strongly than broader community
159 divergence (MPD; Fig. 3). While chemical dissimilarity increased with MPD among communities
160 with low functional or phylogenetic divergence (e.g., comparisons among ruderal communities),
161 the relationship weakened with increasing MPD but remained strong across the full range of
162 MNTD values. Functional and phylogenetic composition explained similar proportions of chemical
163 variation overall, with consistently stronger effects of MNTD than MPD (Fig. S5). At the species
164 level, however, increasing functional and phylogenetic distances were associated with greater
165 chemical divergence (Fig. S6).

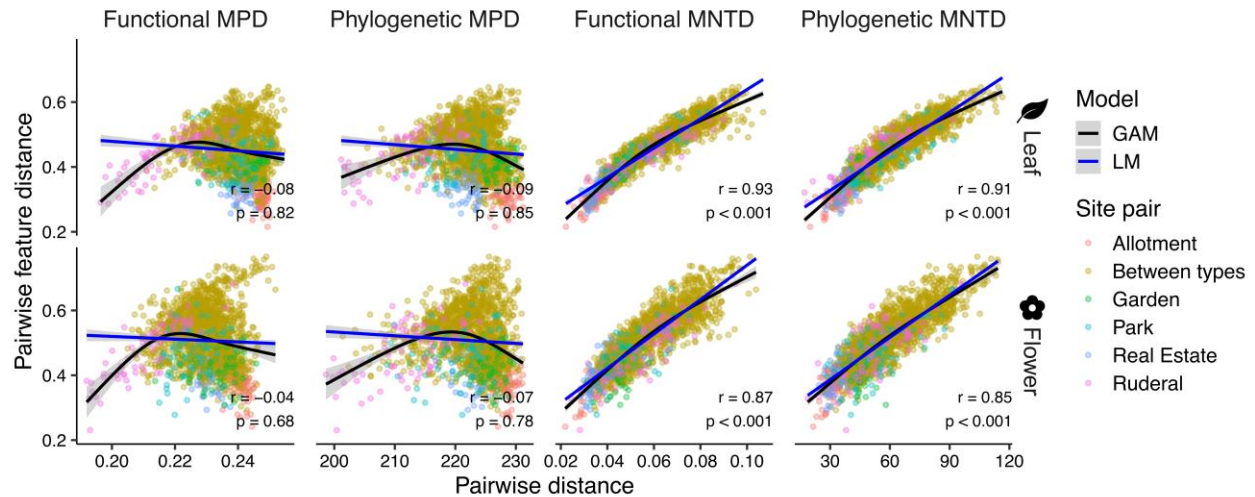


Figure 3. Relationships between pairwise community dissimilarities in plant traits, phylogenetic composition, and pairwise chemical feature composition for leaf- (top) and flower-associated metabolites (bottom). Each point represents a pairwise community comparison, with colors indicating comparisons within or between UGS types. Columns show mean pairwise distance (MPD), representing overall functional or phylogenetic dissimilarity, and mean nearest taxon distance (MNTD), representing finer-scale dissimilarity. Blue and black lines show linear regression (LM) and generalized additive models (GAM), respectively, with 95% confidence intervals. Insets at the bottom right of each subplot report Mantel test results.

Plant traits underlying urban phytochemical signatures

To identify the plant traits associated with phytochemical composition, we used partial least squares (PLS) regression to link community-level trait composition, summarized as community-weighted means for continuous traits and proportional representation of categorical traits, with site-level metabolomic profiles by constructing latent variables (i.e., components) that maximize their shared covariance. The contribution of individual traits to these trait–chemistry relationships was quantified using variable importance in projection (VIP) scores. PLS revealed that differences in phytochemical composition among urban green-space types were associated with distinct combinations of plant traits (Fig. 4). Phytochemical profiles of ruderal sites were characterized by

184 disturbance-associated traits, including ruderal or stress-tolerant strategies (Table S1), but also
185 yellow flowers, bilateral symmetry, and extended flowering periods, whereas phytochemical
186 composition in allotments was associated with a greater contribution of non-native species. Other
187 UGS types showed weaker separation, although human-associated traits, particularly growth form
188 for leaf metabolomes and leaf morphology for floral chemistry, were among the strongest
189 predictors of phytochemical composition. Human-associated and broader ecological traits
190 contributed similarly to variation in leaf- and flower-associated metabolites, with several trait–
191 chemistry associations shared across plant organs, such that traits from one organ (e.g., leaves)
192 explained chemical variation in the other (e.g., flowers; Fig. 4).

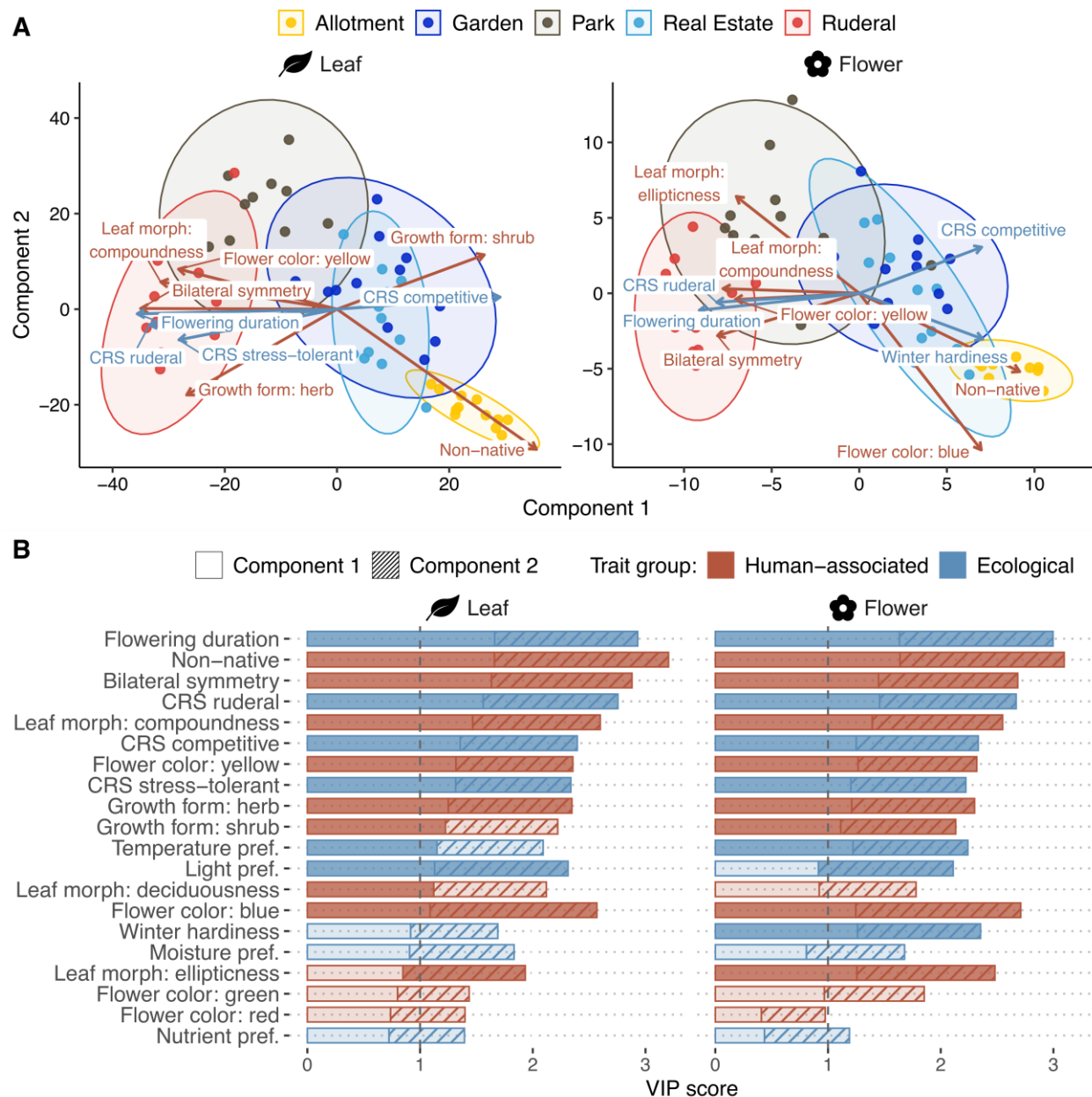


Figure 4. Partial least squares (PLS) analyses linking site-level metabolomic composition with plant functional traits for leaf- and flower-associated metabolites. (A) PLS ordinations of leaf- (left) and flower-associated (right) metabolites. Points represent sampling sites colored by urban green space type; ellipses indicate 95% confidence intervals of group dispersion. Arrows show the direction and magnitude of the 10 most influential traits based on VIP scores from the first PLS component, with colors distinguishing human-associated (red) and ecological trait (blue) categories. (B) VIP scores for the top 20 trait predictors across the first two PLS components. Solid and striped patterns indicate Components 1 and 2, respectively; colors denote human-associated

versus ecological traits. The dashed line marks the $VIP = 1$ threshold; traits above this value are considered influential predictors, whereas lighter-shaded traits indicate lower relative importance.

Increasing human influence enhances phytochemical diversity through community assembly

To distinguish direct effects of human influence on phytochemical richness from those mediated through community assembly, we first modelled relationships between the human-influence index and taxonomic, functional, phylogenetic and chemical diversity. This approach revealed that human influence was positively associated with the richness of both leaf- and flower-associated metabolites, with no evidence of saturation across the observed gradient (Fig. 5A), and similarly increased taxonomic, functional and phylogenetic diversity (Fig. S7). We then integrated these relationships using piecewise structural equation models (SEMs) to quantify direct and indirect pathways linking human influence, functional diversity, phylogenetic structure and chemical richness. SEMs showed that the positive association between human influence and phytochemical richness was primarily mediated by functional richness, representing the extent of functional trait space occupied by communities (Fig. 5B, C). Human influence consistently increased functional richness of both human-related and broader ecological traits, which in turn increased both leaf- and flower-associated metabolite richness. Human influence also increased MPD, but not MNTD, indicating contrasting responses across phylogenetic scales. While MNTD was the strongest predictor of phytochemical composition (Fig. 3), phytochemical richness was positively associated with MPD and negatively associated with MNTD (Fig. 5B,C). These relationships were largely consistent across leaf- and flower-associated metabolites, although flower metabolite richness was more strongly associated with human-related than broader ecological traits.

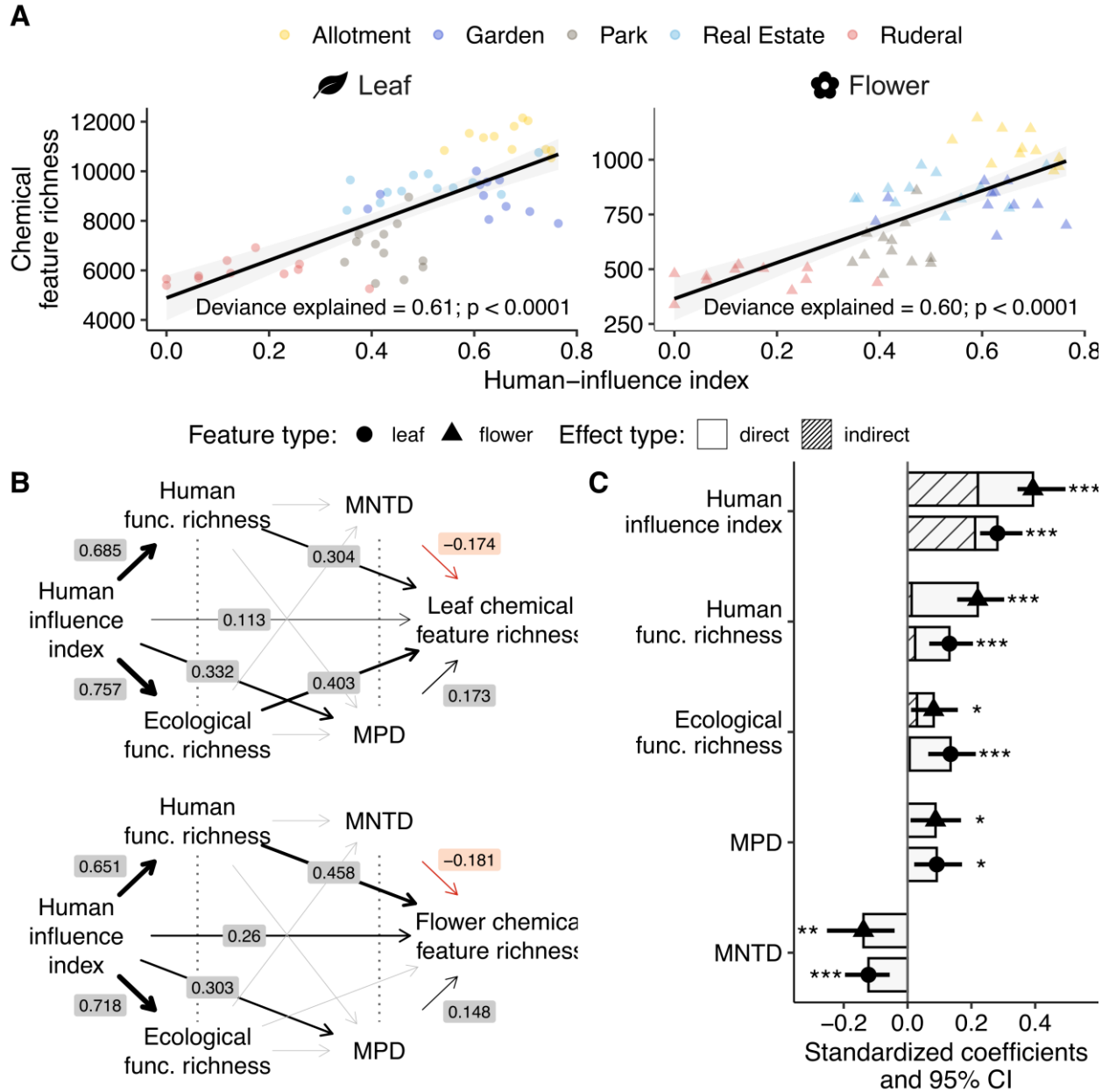


Figure 5. Effects of human influence on the chemical, functional, and phylogenetic diversity of leaf and flower assemblages. (A) Linear relationships between the human-influence index and chemical feature richness of leaf- (left) and flower-associated metabolites (right). Points represent sampling sites (color-coded by UGS type). Insets denote results of generalized linear models, with values indicating deviance explained. (B) Structural equation models describing direct and indirect effects of human influence on chemical feature richness via functional trait and phylogenetic diversity for leaf- (top) and flower-associated metabolites (bottom). Arrows show standardized path coefficients, with width proportional to effect size. Colors indicate effect direction (black = positive, red = negative, grey = non-significant), and dotted lines denote correlated residuals. (C)

Bootstrapped standardized total (points $\pm$ 95% CI), direct (solid bars), and indirect (striped bars) effects on chemical feature richness. Circles and triangles denote leaf- and flower-associated metabolites, respectively. Symbols indicate significance (= $p < 0.05$; ** = $p < 0.01$; *** = $p < 0.001$). MNTD = mean nearest taxon distance; MPD = mean pairwise distance.*

Discussion

We investigated whether human-mediated plant community assembly restructures urban phytochemical landscapes, whether such restructuring is associated with functional and phylogenetic shifts, and whether traits associated with human preferences contribute to these patterns. By integrating plant community surveys encompassing 539 plant species with untargeted metabolomics, functional traits, and phylogenetic information, we show that human-mediated community assembly is associated with a marked reorganization of the chemical dimension of plant biodiversity. Functional, phylogenetic, and phytochemical composition shifted in parallel across urban green spaces, yet chemical turnover remained sensitive to species replacement even when communities differed little in their broader functional or evolutionary structure (i.e., low MPD). At the same time, increasing human influence was associated with greater phytochemical richness, largely through increases in plant functional diversity. Together, these results suggest that phytochemical diversity is not only a property of individual species but also emerges as a feature of community assembly: changes in species composition alter both the identity and the breadth of the chemical environments generated by plant communities.

The parallel shifts in functional, phylogenetic and phytochemical composition indicate that the social-ecological filters structuring urban plant communities extend to their chemistry^{20,30,31}. Ruderal areas and allotments occupied particularly distinct regions of these multidimensional spaces, consistent with contrasting assembly processes dominated by spontaneous colonization and

environmental filtering in the former and deliberate planting in the latter^{25,32,33}. Parks, real-estate areas and private gardens exhibited more gradual transitions, likely because their multiple functions (e.g., recreation, human well-being, cooling) promote a wider range of planting and management practices^{8,23,25}. Importantly, these patterns were consistent across leaf- and flower-associated metabolites, suggesting that human activities reshape broad phytochemical profiles rather than isolated chemical pathways³⁴. These parallel responses likely reflect the broad phylogenetic breadth introduced by human plantings, which may overshadow the organ-specific evolutionary patterns shaped by interactions with pollinators and herbivores in more natural communities (e.g.,^{13,14}). From the perspective of organisms responding to plant chemistry, cities may consequently represent not only mosaics of habitats^{2,35}, but also mosaics of chemically distinct plant communities.

A particularly striking result was that phytochemical differentiation did not require broad functional or phylogenetic divergence. Chemical dissimilarity was more consistently associated with fine-scale differences captured by nearest-neighbor distances (MNTD) than with broad differences among evolutionary or functional assemblages. Urban floras across sites often share representation of major plant lineages (e.g., monocots vs dicots), while differing in the species representing those lineages^{36–38}. This reveals a potential mismatch between human perceptions of vegetation change and ecological consequences: small-scale species replacements, such as replacing one ornamental species with a closely related species, may appear negligible from a human perspective³⁹, yet can already alter the chemical cues available to herbivores, pollinators, and other organisms^{10,11}. Species substitutions that appear functionally redundant from a coarse trait or phylogenetic perspective may therefore not be chemically redundant^{9,10}. Consequently, our findings highlight that functional and phylogenetic diversity cannot necessarily be used as complete surrogates for the chemical dimension of biodiversity.

In practice, however, planting decisions are rarely guided by the broader functional, phylogenetic or phytochemical combinations that species contribute, but are often shaped by their visible characteristics and perceived functions ^{21,22,40}. The association between conspicuous, human-related traits and chemical composition suggests that the observed associations are consistent with aesthetic selection contributing to phytochemical differentiation. Although visual traits are unlikely to directly regulate metabolism ⁴¹, they may act as proxies for broader ecological syndromes linking functional, phylogenetic and phytochemical composition ^{42,43}. This is supported by the shared trait predictors of leaf- and flower-associated metabolites, indicating that selection on individual attributes, such as flower color, can generate coordinated shifts in chemical profiles across plant organs. However, other traits, notably linked to plant persistence in urban settings (e.g., stress tolerance, life-history strategies ⁴⁴), also contributed to chemical differentiation. Although these traits may covary with visually selected characteristics, their association with phytochemical composition may also suggest that environmental filtering can promote distinct chemical strategies independent of human planting decisions. Thus, urban phytochemical composition emerges from both human planting choices and the ecological conditions they create, with both aesthetic preferences and environmental constraints shaping the chemical landscape of cities.

Beyond altering phytochemical composition, human influence consistently increased phytochemical richness, primarily through functional diversification across leaf and flower metabolites. This effect was further reinforced by phylogenetic diversity, with deeper evolutionary lineages supporting richer chemical repertoires. For flower metabolites, however, richness was more strongly associated with human-related trait diversity, consistent with weaker phylogenetic constraints than those on leaf-associated metabolites ^{16,18,19}. Thus, urban planting decisions shape both the identity and breadth of community-level chemistry: replacing species with close relatives can alter chemical composition through differences in metabolite profiles, whereas greater

functional and phylogenetic diversity can increase phytochemical richness by expanding the range of chemical profiles represented within communities. These anthropogenic chemical landscapes may, in turn, expose higher trophic levels to unprecedented mixtures of cues, rewards, and defenses, potentially creating or suppressing interactions compared to non-urban systems⁴⁵. For example, floral volatiles released by one species may attract pollinators or natural enemies that subsequently interact with neighboring species lacking those signaling compounds⁴⁶. Whether this increased chemical diversity reinforces or disrupts established networks remains uncertain and will require tracing how human-driven changes in plant chemistry cascade across trophic levels⁴⁶.

Our study reveals strong links between human influence, community assembly and phytochemical diversity. However, by reconstructing community-level chemistry from species presence, we captured broad patterns of urban phytochemical variation but overlooked how abundance, biomass and local environmental conditions modulate metabolite production^{47,48}. Future studies integrating abundance data and repeated measurements of individuals across environmental gradients are needed to disentangle the relative contributions of plant community composition and environmental conditions⁴⁹. This is particularly important in cities, where microclimate, soil properties, and management practices can vary extensively across social, cultural, and economic contexts^{2,30,35}. Our approach also likely underestimated intraspecific chemical variation, especially for flower metabolites, where logistical constraints limit replication for most species. While sampling all individuals was unfeasible (>500 plant species across 60 sites), we accounted for intraspecific variability in leaf chemistry and assessed limited intraspecific variation in flower metabolites (see *Supplementary Materials I*). Yet, we acknowledge that the contribution of intraspecific variability to urban phytochemical landscapes remains largely unresolved⁵⁰. Finally, our analysis concerns a single city. Testing whether similar patterns emerge across cities differing

in climate, regional flora, cultural preferences, and management traditions will determine how general the relationship between human community assembly and phytochemical diversity is^{32,51}. More broadly, our findings reveal that human modification of biodiversity extends beyond the species and traits that are readily observed. By determining which plants coexist, human decisions and activities can reorganize the chemical repertoires through which plants communicate, defend themselves and interact with other organisms. Moreover, this chemical restructuring can occur through species replacements that leave relatively weak signatures in broad functional or phylogenetic metrics. Phytochemical diversity therefore represents a largely hidden axis of biodiversity change that complements taxonomic, functional, and phylogenetic perspectives. Incorporating this chemical dimension into community ecology may provide a more complete understanding of how human-driven assembly reshapes the ecological interactions and functions that emerge from biological communities.

Methods

Study system and sampling design

We conducted the study in Zurich, Switzerland (445,000 inhabitants; 2024 census), a densely urbanized landscape comprising diverse public and private green spaces. Following the UGS framework of Swan et al.^{2,23}, we selected five UGS types representing contrasting levels and forms of human influence: ruderal areas, parks, green spaces managed by residential estates (henceforth, “real estate”), private gardens, and allotments. These UGS types capture major forms of urban vegetation and levels of human-driven assembly processes: ruderal areas are secondary grasslands and meadows, characterized by low management intensity (typically one to three mowing events per year) and spontaneous, stress-tolerant vegetation, whereas allotment gardens are dominated by

intentionally planted species selected for food production or ornamental purposes and strongly shaped by gardeners' preferences^{25,32}. Parks, real-estate areas and private gardens represent intermediate conditions, where vegetation is typically initially human-selected but subsequent management ranges from low-intensity maintenance allowing spontaneous colonization to intensive horticultural practices^{8,23,25}.

Within each UGS type, we selected 12 sites (60 sites in total) along orthogonal gradients of urbanization and habitat structural complexity (Fig. S1). Urbanization was quantified as the proportion of impervious surface within a 500 m buffer, while structural complexity was characterized by lawn cover and the diversity of habitats (meadows, shrublands, trees, flower beds, agricultural areas and wetlands) within each UGS. This design ensured that each green-space type was represented across a broad range of environmental conditions (Fig. S1). Further details on site selection are available in Casanelles-Abella et al.³².

Finally, we quantified human influence on UGS management using a validated 42-item questionnaire adapted from Tresch et al.²⁸ and completed by local managers. Following Ruile et al.,²⁵, responses were summarized into a human-influence index integrating manager investment, a proxy for ecological stewardship²⁹. Higher index values indicate greater time and effort devoted to managing green spaces. This index was also positively correlated with indicators of both increased disturbance intensity (e.g., mowing and pruning; Pearson's $r = 0.68$; $p < 0.001$) and biodiversity-oriented management practices (e.g., reduced pesticide use; $r = 0.30$; $p = 0.02$), thereby capturing a gradient of human influence on UGS management. Details on index calculation are provided in Ruile et al.²⁵.

Plant and trait data acquisition

Plant communities were surveyed along transects at each site during three sampling periods: April–May, May–June and June–August 2024, covering the phenology of most of Zurich’s urban flora²⁶. The number of transects was scaled to habitat heterogeneity, while total sampled area was standardized to 100 m² per site. In allotment gardens, transects covered the entire site; in private gardens, sampling was divided equally between central and peripheral areas; in ruderal areas, transects were placed randomly; and in parks and real estate areas, transects followed mapped habitat proportions, excluding habitats covering <5% of the site³². Detailed sampling procedures are provided in Ruile et al.²⁶.

Species-level trait information was compiled from published databases, following Grothe et al.²⁷. We selected 26 functional traits (sensu Violle et al.⁵²) considered to influence plant selection and survival in cities, and classified them into two groups representing pathways through which human preferences shape plant communities (e.g.,^{22,40,53}): (i) human-associated traits: 11 traits related to growth form, plant height, floral characteristics, leaf morphology and coloration, and species origin, all of which are likely to influence human perception and management decisions; and (ii) broader ecological traits, including 15 traits describing environmental preferences, physiology, and life-history strategies (Table S1 provides the source, definition, and classification and associated literature for all traits). Although these groups provide a conceptual framework for our hypotheses, we acknowledge that trait–preference associations may vary across cultural contexts and therefore also report individual trait effects independently of this classification.

Metabolomic characterization

We characterized plant chemical diversity separately for leaf metabolites and flower volatiles. Leaf metabolomes were obtained for 416 plant species, whereas floral volatiles were characterized for 380 species (henceforth, leaf- and flower-associated metabolites, respectively; 257 species shared

across datasets). Analyses were restricted to angiosperms (clade Angiospermae), excluding conifers, ferns, mosses, and other non-flowering species. To account for intraspecific variation, leaf metabolomes were characterized from five individuals per species, collected at different sites, and pooled before extraction. Due to logistical constraints, flower-associated metabolite profiles could only be obtained from a single flowering individual per species. Nevertheless, replicate sampling across the most common species indicated that intraspecific variation was substantially lower than interspecific variation, supporting the use of species-level chemical profiles (see *Supplementary Material I; Fig. S8*).

Flower volatile organic compounds

For each plant in full bloom (species = 380), a fresh flower or inflorescence (samples = 416) was collected and placed in individual 20 mL analytical glass vials closed with a metallic cap with a silicone/PTFE septum. Field samples were kept at 4°C before being frozen at -80°C by the end of the collection day. Before chemical analysis, 200 ng of an internal standard were added to each defrosted sample (naphthalene, CAS# 91-20-3, Sigma-Aldrich, mixed in 2 µL dichloromethane, CAS# 75-09-2, Honeywell GmbH).

Volatile collection was carried out using a multipurpose robotic sampler (MPS, Gerstel GmbH) and a solid phase microextraction (SPME) Arrow fiber (polydimethylsiloxane phase (PDMS), 100 µm thickness, 1.1 mm diameter, 20 mm length, PAL System CTC Analytics AG). The flower sample was placed in an incubator-agitator for 1 min (35°C, 250 rpm stirring), then the SPME fiber was inserted through the septum. The PDMS phase was allowed to trap VOCs released into the headspace for 15 min at 35°C, stirring at 120 rpm. Pre- and post-sampling bake-out of the SPME fiber were carried out (250°C, 2 and 4 min, respectively).

All VOCs were analyzed using an Agilent 8890 gas chromatograph (GC) coupled to an Agilent 5977B mass spectrometer detector (Agilent Technologies, Santa Clara, CA, USA). The SPME fiber was thermally desorbed for 3.5 min in the GC front injector set at 250 °C in splitless mode (total flow 64 mL min⁻¹, 13.3 psi pressure, helium carrier gas). In the GC, the volatiles were separated on a semi-standard non-polar column (HP5-ms Ultra Inert; 30 m length, 0.25 mm internal diameter, 0.25 µm film thickness; J & W Scientific, Agilent Technologies). In the oven, the column temperature was kept at 40 °C for 2 min, then ramped up to 260 °C at 7 °C min⁻¹ (hold 1 min), followed by a 2 min post run at 270 °C. Helium at a constant flow mode of 1.0 mL min⁻¹ was used as a carrier gas. In all the analyses, the MSD transfer line temperature was set at 280 °C, and the ion source and quadrupole temperatures were set at 230 °C and 150 °C, respectively. Electron impact (EI, ionization potential 70 eV) mode was used with scanning over the mass range of 33–350 m/z.

The chromatogram outputs were exported as raw .CDF data and processed in MzMine V.3⁵⁴ for mass and feature detection (centroid, signal-to-noise threshold S/N>3 and ADAP builder at m/z tolerance 0.500), peak picking (ADAP resolving with height 600, area threshold 50, RT wavelet range 0.00 - 0.03), deconvolution (hierarchical clustering, excluded m/z values 73, 207, 208), alignment (ADAP aligner, min confidence 0.1, RT tolerance 0.6, m/z tolerance 1)⁵⁵. The resulting samples (416) × features (3161) table was then cleaned from all obvious contaminants (e.g., analytical equipment, industry, cosmetics, air pollutants, insecticides). Another round was carried out to discard all features related to compounds unknown to be emitted by plants, resulting in a final samples (416) × features (1822) set.

Non-volatile metabolite extraction and LC–MS profiling

440 Leaf samples were oven-dried at 60 °C for 72 hours, milled to a fine powder, and extracted (20 mg
441 dry weight) in 1 mL of water–methanol–formic acid (30:69.9:0.1). Extracts were centrifuged
442 (14,000 g, 5 min), and supernatants were collected, re-centrifuged, and transferred to vials for LC–
443 MS analysis. Aqueous methanolic leaf extracts of each plant species sample were analyzed by
444 ultra-high performance liquid chromatography - quadrupole time-of-flight mass spectrometry
445 (UHPLC-QTOFMS) using an Acquity UPLC™ I-Class coupled to a Synapt XS (Waters, Milford,
446 USA) ⁵⁶. The system was controlled by MassLynx v.4.2. An Acquity UPLC™ HSS T3 column
447 (100 × 2.1 mm, 1.8 µm) maintained at 25 °C was used at a flow rate of 0.5 ml/min. Mobile phases
448 consisted of H₂O + 0.05% formic acid (solvent A) and acetonitrile + 0.05% formic acid (solvent
449 B). A linear gradient from 0 to 100% B in 10.0 min was applied. The injection volume was 0.5 µl.
450 MS detection was performed in negative electrospray ionization and using data-dependent
451 acquisition (DDA). The resolution was set to 22,000 (at m/z 554). Data were acquired in continuum
452 mode. The capillary voltage was set to -1.0 kV, the cone voltage to -25 V, the source temperature
453 to 140 °C, the desolvation temperature to 500 °C, the desolvation gas flow to 1000 L/h, the cone
454 gas flow to 150 L/h, the nebulizer gas flow to 6.5 bars, and the collision gas (Ar) flow to 2.0 L/min.
455 DDA settings were as follows: MS1 mass range and scan time 50–1200 Da and 0.1 s, respectively,
456 top 7 MS/MS (0.05 s scan time each), intensity threshold 15,000 counts per s, MS/MS selection
457 window 4 Da, peak deisotoping activated, dynamic exclusion of 1.5 s after acquisition. An
458 exclusion list of the 150 most intense background ions was generated from a blank sample run just
459 before the plant samples. For MS/MS acquisition, a ramped collision energy of 5-40 V (at m/z 50)
460 and 20-70 V (at m/z 1200) was set. Quality control samples were prepared by pooling aliquots of
461 all samples and run 4 times before the batch and about every 30 samples during the batch.

462 Feature detection in MzMine V.3 ⁵⁴ was performed using noise levels for MS1 and MS2 of 1500
463 and 40, respectively. The parameters for ADAP chromatogram builder were: minimum group size

in number of scans 5, group intensity threshold 2000, minimum height intensity 2000, m/z tolerance 0.015 Da or 15 ppm. The chromatogram deconvolution algorithm used was wavelets (ADAP) and parameters were: threshold 10, minimum feature height 1500, coefficient/area threshold 50, peak duration range 0.01-0.5 min, RT wavelet range 0.00-0.06, m/z center calculation median, m/z and RT range for MS2 scan pairing 0.1 and 0.12. The isotope peak grouper parameters were: m/z tolerance 0.015 Da or 15 ppm, retention time tolerance 0.07, maximum number of charges 2, most intense isotope. The joint aligner parameters were: m/z tolerance 0.015 Da or 15 ppm, retention time tolerance 0.1, weight for m/z 50, weight for RT 50. Only features with a minimum of 2 isotopes and MS2 spectra were retained by filtration. No gap-filling was applied.

Data processing and statistical analyses

As an initial step, although already explored by previous studies^{25,26}, we confirmed that plant communities differed in composition among UGS types using principal coordinate analysis (PCoA) based on Jaccard dissimilarities (Fig. S9). We then quantified complementary measures of chemical, functional, and phylogenetic diversity to assess how plant community assembly relates to phytochemical diversity. Site-level chemical composition was reconstructed by pooling all metabolites detected across species occurring at each site, separately for leaf- and flower-associated metabolites (Fig. S1). Because metabolite detection depends on analytical sensitivity and biomass contribution of plant organs, chemical composition was represented as feature presence–absence rather than abundance. Chemical richness was quantified as the number of distinct features, while composition shifts among sites were assessed using Jaccard dissimilarities. We also assessed the relationship between plant and chemical richness, and whether it differed among UGS types, using generalized linear models (GLMs) and Wilcoxon tests (see *Supplementary Material II*).

We reconstructed a species-level phylogeny from the extended GBOTB mega-tree⁵⁷. Phylogenetic structure was quantified using two complementary metrics capturing turnover at different evolutionary scales: mean pairwise distance (MPD), which reflects replacement among distantly related lineages, and mean nearest taxon distance (MNTD), which captures turnover among closely related taxa within the same major lineages⁵⁸. Accordingly, communities differing in dominant clades (e.g., Asparagales vs. Rosales) exhibit high MPD, whereas communities sharing major clades but differing in species composition exhibit high MNTD. We used both metrics to quantify pairwise phylogenetic turnover among sites and within-community phylogenetic diversity. As expected from their complementary evolutionary scales, MPD and MNTD were not significantly correlated ($p > 0.05$). MPD was, however, strongly correlated with other common measures of broad phylogenetic diversity (for example, Faith's PD; leaf: $r = 0.75$; flower: $r = 0.73$; both $p < 0.001$).

Functional composition was quantified from species-level Gower dissimilarities, integrating continuous, ordinal, binary, and categorical traits. Functional shifts among sites were assessed using the same MPD/MNTD framework to capture broad- and fine-scale shifts in trait composition. However, because average pairwise trait distances do not directly describe the extent or distribution of occupied functional space, within-community functional diversity was quantified using functional richness and functional dispersion, which measure the volume of occupied trait space and the distribution of species within it, respectively. All metrics were calculated separately for human-associated and broader ecological traits. Further details on phylogenetic and functional diversity metric calculations are available in *Supplementary Material III*.

Linking community assembly to chemical composition

We first tested whether functional and phylogenetic turnover among communities was associated with chemical composition. Pairwise chemical dissimilarities were related to functional and phylogenetic distances using linear and generalized additive models (GAMs; $k = 4$) to assess both monotonic and nonlinear relationships. Because pairwise distances are not statistically independent, these analyses were complemented by Mantel tests with 9,999 permutations.

To evaluate whether chemical, functional, and phylogenetic composition occupied comparable multivariate spaces, we performed separate PCoAs of chemical, functional (human-associated and broader ecological traits analyzed separately), and phylogenetic dissimilarity matrices for leaf- and flower-associated metabolites. Ordinations were generated using Lingoes correction to obtain Euclidean representations of the dissimilarity matrices. Congruence among ecological spaces was then assessed using Procrustes analyses based on the first two PCoA axes, with significance evaluated using PROTEST permutation tests (9,999 permutations). To assess associations between compositional gradients and the human-influence index, we fitted smooth response surfaces onto the Procrustes ordinations using GAMs ($k = 10$).

Finally, we quantified the unique and shared contributions of functional and phylogenetic composition to chemical composition using distance-based redundancy analysis (db-RDA) and variation partitioning. Chemical composition was modelled against the first two PCoA axes summarizing human-associated traits, broader ecological traits, and phylogenetic composition (six predictors in total), and predictor significance was assessed using 9,999 permutations.

Identifying the traits associated with chemical composition

To identify associations between specific traits and chemical composition, we used partial least squares (PLS) regressions, which identify latent components that maximize covariance between predictor (trait) and response (chemical composition) datasets. Separate models were fitted for leaf-

and flower-associated metabolites. Because PLS requires continuous predictors, species-level traits were converted into community-level descriptors: continuous and ordinal traits were summarized as community-weighted means, whereas categorical traits were represented as the proportion of species expressing each trait state within a community (e.g., the proportion of species with red flowers).

The optimal number of latent components was determined using repeated five-fold cross-validation (1000 iterations) based on total predictive ability (total Q^2). Cross-validation consistently supported a single component ($ncomp = 1$), indicating that most trait–chemistry covariance was captured by one dominant axis (Fig. S10). Models were nevertheless refitted with two components for visualization purposes, although our interpretation remained focused on the first component. Trait contributions were quantified using variable importance in projection (VIP) scores, which summarize the contribution of each predictor to the covariance captured by the PLS model. VIP scores are presented for both components to facilitate comparison with the ordination space, with our interpretation, once again, focusing on the scores associated with the first component only.

Testing pathways linking human management to chemical richness

Finally, we tested whether human management influenced chemical richness directly or indirectly through changes in functional and phylogenetic structure. Chemical richness, as well as functional and phylogenetic diversity metrics, were first modelled individually as functions of the human-influence index using (G)LMs (negative binomial distribution for chemical richness; Gaussian distribution for functional and phylogenetic metrics).

These relationships were subsequently integrated into piecewise structural equation models (SEMs). Separate SEMs were fitted for leaf- and flower-associated metabolites using identical topologies. Models tested whether increasing human influence altered human-associated and

broader ecological trait richness, whether these changes propagated to phylogenetic community diversity (MPD and MNTD), and whether functional richness and phylogenetic diversity ultimately influenced chemical feature richness. Covariances among related functional and phylogenetic diversity metrics, respectively, were included (e.g., covariance between human-associated and broader ecological trait richness). To maintain model parsimony, the pathway between the human-influence index and MNTD was excluded because no association was detected in the individual models (Fig. S7). The resulting model showed good fit (non-significant Fisher's C; Table S2), with all independence claims satisfied (Table S3). Path coefficients were evaluated using bootstrap-derived 95% confidence intervals from 1,000 permutations, allowing us to distinguish direct and indirect pathways linking human influence with chemical richness.

All analyses were conducted using R v4.5.3⁵⁹. The following packages were used in the analysis: *vegan* v2.7-3, *V.PhyloMaker2* v0.1.0, *ape* v5.8-1, *picante* v1.8.2, *mFD* v1.0.7 (biodiversity metric calculations; ^{57,60–63}); *mixOmics* v6.32.0, *piecewiseSEM* v2.3.1, *semEff* v0.7.2 (modeling; ^{64–66}); *qgraph* v1.9.8, *ggplot2* v4.0.2 (visualization; ^{67,68}).

References

1. Aronson, M. F. *et al.* Hierarchical filters determine community assembly of urban species pools. *Ecology* **97**, 2952–2963 (2016).
2. Swan, C. M. *et al.* A framework for understanding how biodiversity patterns unfold across multiple spatial scales in urban ecosystems. *Ecosphere* **12**, e03650 (2021).
3. United Nations. *World Urbanization Prospects: The 2018 Revision*. (United Nations, New York, 2018).
4. Lee, A. C. & Maheswaran, R. The health benefits of urban green spaces: a review of the evidence. *Journal of public health* **33**, 212–222 (2011).
5. Schwarz, N. *et al.* Understanding biodiversity-ecosystem service relationships in urban areas: A comprehensive literature review. *Ecosystem Services* **27**, 161–171 (2017).
6. Kowarik, I. *et al.* Promoting urban biodiversity for the benefit of people and nature. *Nat. Rev. Biodivers.* **1**, 214–232 (2025).
7. Garmendia, E., Apostolopoulou, E., Adams, W. M. & Bormpoudakis, D. Biodiversity and Green Infrastructure in Europe: Boundary object or ecological trap? *Land Use Policy* **56**, 315–319 (2016).
8. Threlfall, C. G. *et al.* Variation in Vegetation Structure and Composition across Urban Green Space Types. *Front. Ecol. Evol.* **4**, (2016).
9. Stevenson, P. C., Nicolson, S. W. & Wright, G. A. Plant secondary metabolites in nectar: impacts on pollinators and ecological functions. *Functional Ecology* **31**, 65–75 (2017).
10. Kessler, A. & Kalske, A. Plant Secondary Metabolite Diversity and Species Interactions. *Annual Review of Ecology, Evolution, and Systematics* **49**, 115–138 (2018).
11. Schwery, O. *et al.* Plant scent and plant–insect interactions—Review and outlook from a macroevolutionary perspective. *Journal of Systematics and Evolution* **61**, 465–486 (2023).

- 593 12. Upadhyay, R., Saini, R., Shukla, P. K. & Tiwari, K. N. Role of secondary metabolites in
594 plant defense mechanisms: a molecular and biotechnological insights. *Phytochem Rev* **24**,
595 953–983 (2025).
- 596 13. Asner, G. P. *et al.* Amazonian functional diversity from forest canopy chemical assembly.
597 *Proceedings of the National Academy of Sciences* **111**, 5604–5609 (2014).
- 598 14. Kantsa, A. *et al.* Community-wide integration of floral colour and scent in a Mediterranean
599 scrubland. *Nat Ecol Evol* **1**, 1502–1510 (2017).
- 600 15. Sedio, B. E. *et al.* Chemical Similarity of Co-occurring Trees Decreases With Precipitation
601 and Temperature in North American Forests. *Front. Ecol. Evol.* **9**, (2021).
- 602 16. Schneider, G. F. & Beckman, N. G. Different tools for different trades: contrasts in
603 specialized metabolite chemodiversity and phylogenetic dispersion in fruit, leaves, and roots
604 of the neotropical shrubs Psychotria and Palicourea (Rubiaceae). *Plant Biology* **27**, 681–697
605 (2025).
- 606 17. Defosse, E. *et al.* Spatial and evolutionary predictability of phytochemical diversity.
607 *Proceedings of the National Academy of Sciences* **118**, e2013344118 (2021).
- 608 18. Sedio, B. E., Parker, J. D., McMahon, S. M. & Wright, S. J. Comparative foliar
609 metabolomics of a tropical and a temperate forest community. *Ecology* **99**, 2647–2653
610 (2018).
- 611 19. Burkle, L. A., Glenny, W. R. & Runyon, J. B. Intraspecific and interspecific variation in
612 floral volatiles over time. *Plant Ecol* **221**, 529–544 (2020).
- 613 20. Ruggeri, A. *et al.* Planting for healthy air: Urban biodiversity enhances natural chemical
614 environments. *Plants, People, Planet* **1**, (2026).

- 615 21. Hoyle, H., Hitchmough, J. & Jorgensen, A. All about the ‘wow factor’? The relationships
616 between aesthetics, restorative effect and perceived biodiversity in designed urban planting.
617 *Landscape and Urban Planning* **164**, 109–123 (2017).
- 618 22. Kendal, D., Williams, K. J. H. & Williams, N. S. G. Plant traits link people’s plant
619 preferences to the composition of their gardens. *Landscape and Urban Planning* **105**, 34–42
620 (2012).
- 621 23. Swan, C. M., Pickett, S. T. A., Szlavecz, K., Warren, P. & Willey, K. T. Biodiversity and
622 Community Composition in Urban Ecosystems: Coupled Human, Spatial, and
623 Metacommunity Processes. *Urban Ecology* 179–186 (2011)
624 doi:10.1093/acprof:oso/9780199563562.003.0021.
- 625 24. Avolio, M. L., Swan, C., Pataki, D. E. & Jenerette, G. D. Incorporating human behaviors
626 into theories of urban community assembly and species coexistence. *Oikos* **130**, 1849–1864
627 (2021).
- 628 25. Ruile, S. *et al.* The human handprint in shaping plant diversity in urban environments.
629 <https://ecoevorxiv.org/repository/view/12695/> (2026).
- 630 26. Ruile, S. *et al.* A comprehensive dataset on plant-associated invertebrates and gardening
631 activities, from 100 sites across five urban green space types in Zurich, Lugano, and
632 Geneva, Switzerland. <https://ecoevorxiv.org/repository/view/13826/> (2026).
- 633 27. Grothe, V. *et al.* The Human-Imprinted Regional Species Pool: Functional Trait Patterns of
634 Commercial and Established Plants. *Authorea*
635 <https://doi.org/10.22541/authorea.15003231/v1> (2026) doi:10.22541/authorea.15003231/v1.
- 636 28. Tresch, S. *et al.* Litter decomposition driven by soil fauna, plant diversity and soil
637 management in urban gardens. *Science of The Total Environment* **658**, 1614–1629 (2019).

- 638 29. Bennett, N. J. *et al.* Environmental Stewardship: A Conceptual Review and Analytical
639 Framework. *Environmental Management* **61**, 597–614 (2018).
- 640 30. Aronson, M. F. *et al.* Biodiversity in the city: key challenges for urban green space
641 management. *Frontiers in Ecology and the Environment* **15**, 189–196 (2017).
- 642 31. Augustinus, B. A., Abegg, M., Queloz, V. & Brockerhoff, E. G. Higher tree species richness
643 and diversity in urban areas than in forests: Implications for host availability for invasive
644 tree pests and pathogens. *Landscape and Urban Planning* **250**, 105144 (2024).
- 645 32. Casanelles-Abella, J. *et al.* Social-ecological signatures in plant species composition across
646 Swiss cities and urban green space types. *Plants, People, Planet* **1**, (2026).
- 647 33. Zhao, J. *et al.* Plant species composition in green spaces within the built-up areas of Beijing,
648 China. *Plant Ecol* **209**, 189–204 (2010).
- 649 34. Jamieson, M. A. *et al.* Global change effects on plant–insect interactions: the role of
650 phytochemistry. *Current Opinion in Insect Science* **23**, 70–80 (2017).
- 651 35. Lepczyk, C. A. *et al.* Biodiversity in the City: Fundamental Questions for Understanding the
652 Ecology of Urban Green Spaces for Biodiversity Conservation. *BioScience* **67**, 799–807
653 (2017).
- 654 36. Dylewski, Ł., Banaszak-Cibicka, W., Maćkowiak, Ł. & Dyderski, M. K. How do
655 urbanization and alien species affect the plant taxonomic, functional, and phylogenetic
656 diversity in different types of urban green areas? *Environ Sci Pollut Res* **30**, 92390–92403
657 (2023).
- 658 37. Knapp, S. *et al.* Phylogenetic and functional characteristics of household yard floras and
659 their changes along an urbanization gradient. *Ecology* **93**, S83–S98 (2012).

- 660 38. Knapp, S., Kühn, I., Schweiger, O. & Klotz, S. Challenging urban species diversity:
661 contrasting phylogenetic patterns across plant functional groups in Germany. *Ecology*
662 *Letters* **11**, 1054–1064 (2008).
- 663 39. Faeth, S. H., Bang, C. & Saari, S. Urban biodiversity: patterns and mechanisms. *Annals of*
664 *the New York Academy of Sciences* **1223**, 69–81 (2011).
- 665 40. Goodness, J. Urban landscaping choices and people's selection of plant traits in Cape Town,
666 South Africa. *Environmental Science & Policy* **85**, 182–192 (2018).
- 667 41. Önder, S., Tonguç, M., Erbaş, S., Önder, D. & Mutlucan, M. Investigation of phenological,
668 primary and secondary metabolites changes during flower developmental of *Rosa*
669 *damascena*. *Plant Physiology and Biochemistry* **192**, 20–34 (2022).
- 670 42. Rasmann, S., Pellissier, L., Defosse, E., Jactel, H. & Kunstler, G. Climate-driven change in
671 plant–insect interactions along elevation gradients. *Functional Ecology* **28**, 46–54 (2014).
- 672 43. Wink, M. Evolution of secondary metabolites from an ecological and molecular
673 phylogenetic perspective. *Phytochemistry* **64**, 3–19 (2003).
- 674 44. Williams, N. S. G., Hahs, A. K. & Vesk, P. A. Urbanisation, plant traits and the composition
675 of urban floras. *Perspectives in Plant Ecology, Evolution and Systematics* **17**, 78–86 (2015).
- 676 45. Meiners, T. Chemical ecology and evolution of plant–insect interactions: a multitrophic
677 perspective. *Current Opinion in Insect Science* **8**, 22–28 (2015).
- 678 46. Randlkofer, B., Obermaier, E., Hilker, M. & Meiners, T. Vegetation complexity—The
679 influence of plant species diversity and plant structures on plant chemical complexity and
680 arthropods. *Basic and Applied Ecology* **11**, 383–395 (2010).
- 681 47. Scherling, C., Roscher, C., Giavalisco, P., Schulze, E.-D. & Weckwerth, W. Metabolomics
682 Unravel Contrasting Effects of Biodiversity on the Performance of Individual Plant Species.
683 *PLOS ONE* **5**, e12569 (2010).

48. Yang, L. *et al.* Response of Plant Secondary Metabolites to Environmental Factors. *Molecules* **23**, 762 (2018).
49. Ogwu, M. C., Izah, S. C. & Joshua, M. T. Ecological and environmental determinants of phytochemical variability in forest trees. *Phytochem Rev* **24**, 5109–5137 (2025).
50. Palmer-Young, E. C. *et al.* Chemistry of floral rewards: intra- and interspecific variability of nectar and pollen secondary metabolites across taxa. *Ecological Monographs* **89**, e01335 (2019).
51. Kendal, D., Williams, N. S. G. & Williams, K. J. H. A cultivated environment: Exploring the global distribution of plants in gardens, parks and streetscapes. *Urban Ecosyst* **15**, 637–652 (2012).
52. Violle, C. *et al.* Let the concept of trait be functional! *Oikos* **116**, 882–892 (2007).
53. Hůla, M. & Flegr, J. What flowers do we like? The influence of shape and color on the rating of flower beauty. *PeerJ* **4**, e2106 (2016).
54. Schmid, R. *et al.* Integrative analysis of multimodal mass spectrometry data in MZmine 3. *Nat Biotechnol* **41**, 447–449 (2023).
55. Pluskal, T., Castillo, S., Villar-Briones, A. & Orešič, M. MZmine 2: Modular framework for processing, visualizing, and analyzing mass spectrometry-based molecular profile data. *BMC Bioinformatics* **11**, 395 (2010).
56. Defosse, E., Bourquin, J., von Reuss, S., Rasmann, S. & Glauser, G. Eight key rules for successful data-dependent acquisition in mass spectrometry-based metabolomics. *Mass Spectrometry Reviews* **42**, 131–143 (2023).
57. Jin, Y. & Qian, H. V. PhyloMaker2: An updated and enlarged R package that can generate very large phylogenies for vascular plants. *Plant Diversity* **44**, 335–339 (2022).

- 707 58. Tucker, C. M. *et al.* A guide to phylogenetic metrics for conservation, community ecology
708 and macroecology. *Biological Reviews* **92**, 698–715 (2017).
- 709 59. R Core Team. R: A language and environment for statistical computing. *R Foundation for*
710 *Statistical Computing, Vienna, Austria.* (2025).
- 711 60. Kembel, S. W. *et al.* picante: Integrating Phylogenies and Ecology. (2026).
- 712 61. Magneville, C. *et al.* mFD: Compute and Illustrate the Multiple Facets of Functional
713 Diversity. 1.0.7 <https://doi.org/10.32614/CRAN.package.mFD> (2026).
- 714 62. Oksanen, J. *et al.* vegan: Community Ecology Package. 2.7-5
715 <https://doi.org/10.32614/CRAN.package.vegan> (2026).
- 716 63. Paradis, E. *et al.* ape: Analyses of Phylogenetics and Evolution. 5.8–1
717 <https://doi.org/10.32614/CRAN.package.ape> (2026).
- 718 64. Lefcheck, J., Byrnes, J. & Grace, J. piecewiseSEM: Piecewise Structural Equation
719 Modeling. 2.3.1 <https://doi.org/10.32614/CRAN.package.piecewiseSEM> (2026).
- 720 65. Murphy, M. V. semEff: Automatic Calculation of Effects for Piecewise Structural Equation
721 Models. 0.7.2 <https://doi.org/10.32614/CRAN.package.semEff> (2026).
- 722 66. Rohart, F., Gautier, B., Singh, A. & Cao, K.-A. L. mixOmics: An R package for ‘omics
723 feature selection and multiple data integration. *PLOS Computational Biology* **13**, e1005752
724 (2017).
- 725 67. Epskamp, S., Costantini, G., Haslbeck, J. & Isvoranu, A. qgraph: Graph Plotting Methods,
726 Psychometric Data Visualization and Graphical Model Estimation. 1.10.1
727 <https://doi.org/10.32614/CRAN.package.qgraph> (2026).
- 728 68. Wickham, H. *et al.* ggplot2: Create Elegant Data Visualisations Using the Grammar of
729 Graphics. (2026).

Author contributions

KP, SRa, and MM conceived and designed the study. MM led the funding acquisition for the PAPPUS project (www.wsl.ch/pappus_en). SRu and MM conducted field work. SRa and GR performed chemical analyses and bioinformatic processing. KP analyzed the data, produced the figures, and wrote the initial draft. All authors provided critical comments on previous versions of the manuscript and contributed to writing the final version.

Data availability

Data and code is available on GitHub (https://github.com/KPerrelet/human_phytochemical_assembly) and Zenodo (<https://doi.org/10.5281/zenodo.23493185>).

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Declaration of competing interest

750 The authors declare that they have no known competing financial interests or personal relationships
751 that could have appeared to influence the work reported in this paper.

**Supplementary Material for “Human-mediated community assembly reshapes urban
phytochemical diversity”**

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784 *compound profiles*

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786 *chemical feature richness*

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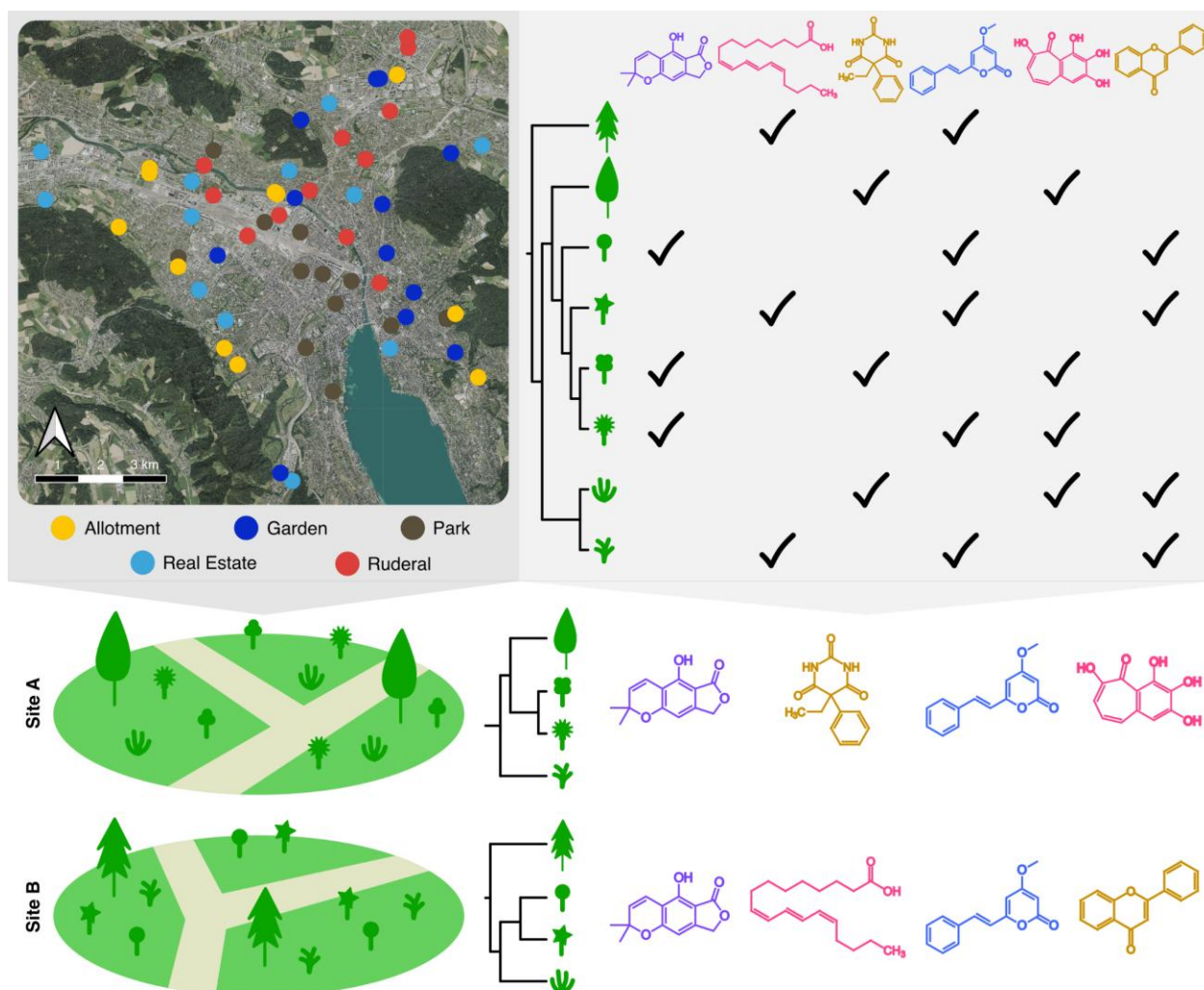


Figure S1. Sampling design and reconstruction of site-level chemical composition. Study sites ($n = 60$) were distributed across five UGS types in Zurich (allotment, garden, park, real estate, and ruderal). Site-level chemical profiles were reconstructed by pooling metabolite features detected across all plant species recorded at each site; the bottom panel illustrates this for two example sites differing in species composition. Plant communities were also used to derive site-level functional (not represented) and phylogenetic (represented here through phylogenetic trees) composition, enabling consistent comparisons among chemical, functional, and phylogenetic dimensions. The molecules shown are illustrative examples.

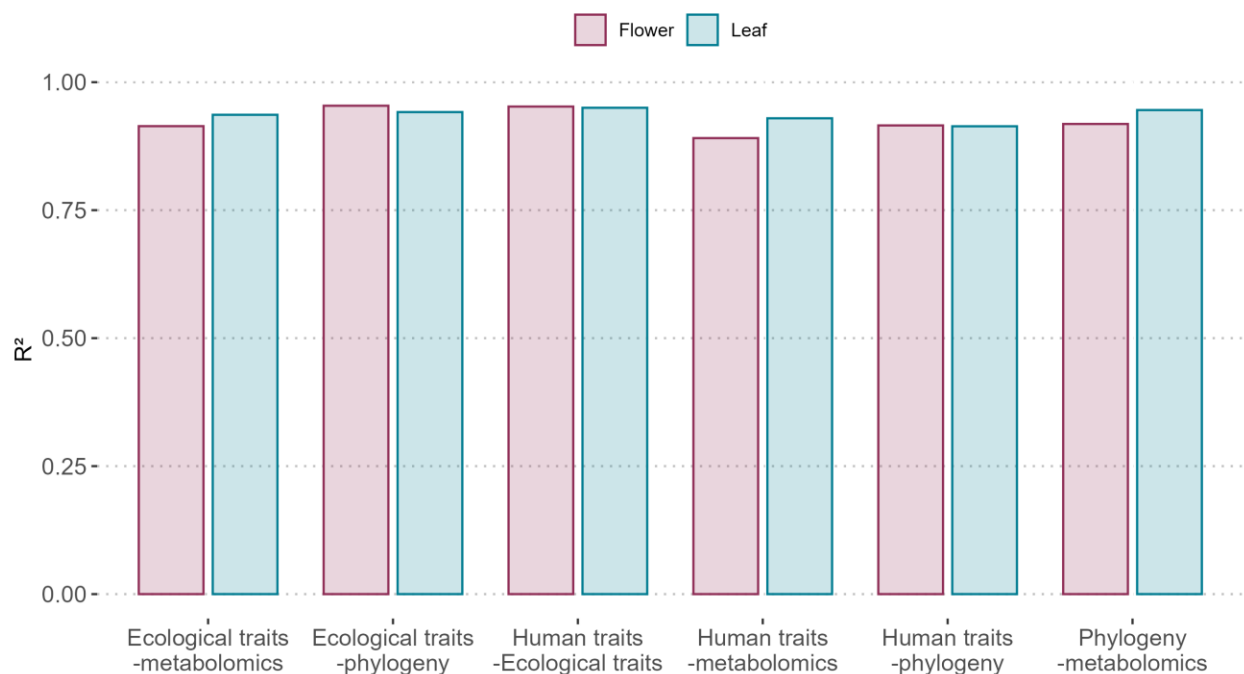


Figure S2. Procrustes correlations between ordinations of chemical, phylogenetic, and functional composition across UGS for leaf- and flower- associated metabolites (color-coded). Bars represent the squared Procrustes correlation (R^2) for pairwise comparisons between human-associated traits, broader ecological traits, phylogeny, and metabolomic composition. All Procrustes correlations were highly significant ($p < 0.001$), with significance assessed using 9,999 permutations.

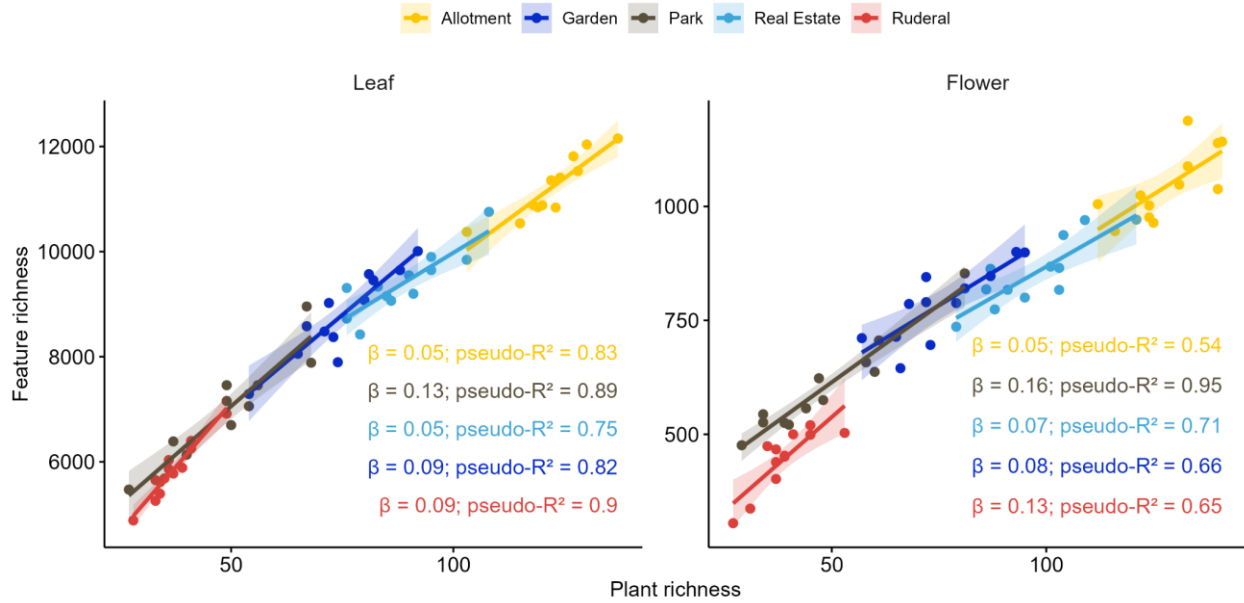
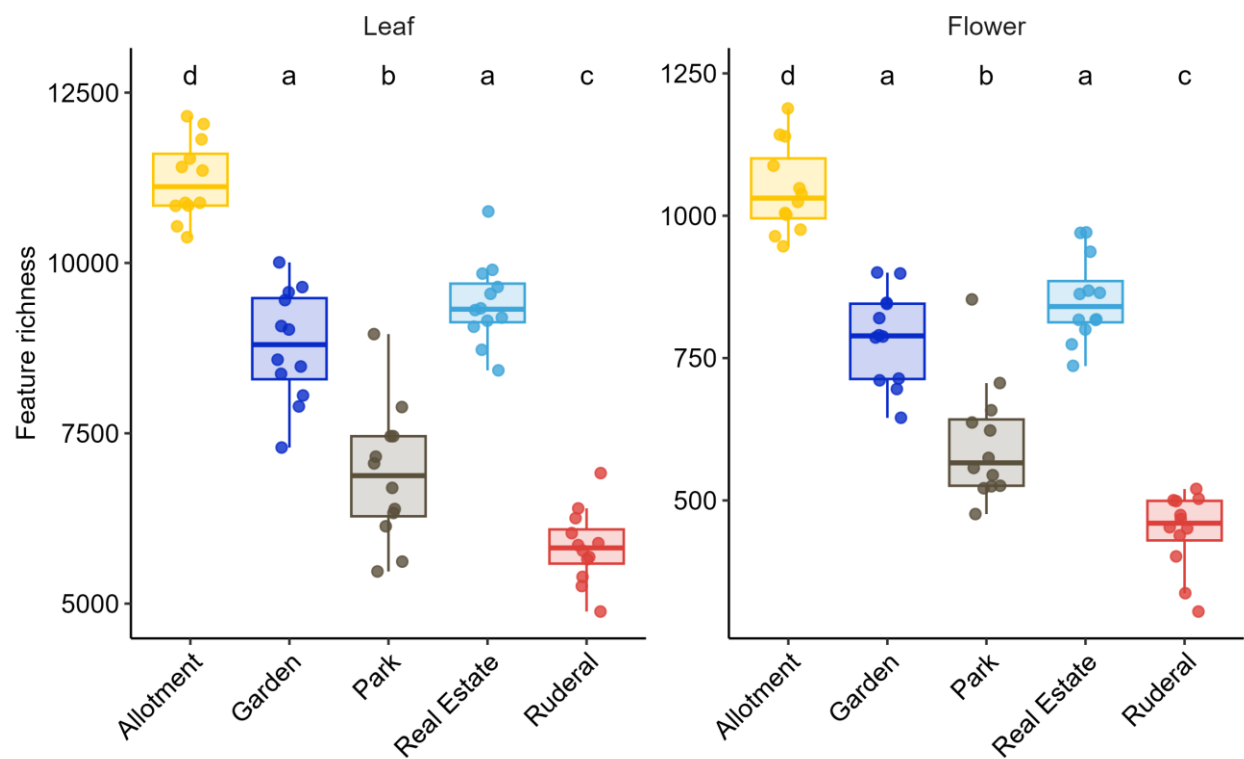


Figure S3. Relationships between plant species richness and chemical feature richness in UGS for leaf- (left) and flower-associated metabolites (right). Points represent individual sites, and lines show linear regression fits. Annotations report β coefficients and pseudo-R² from generalized linear models relating chemical feature richness to standardized plant richness within each UGS type.



807 **Figure S4.** Chemical feature richness across UGS types for leaf- (left) and flower- associated
808 metabolites (right). Points represent individual sites, and different letters indicate significant
809 differences among UGS types based on pairwise Wilcoxon tests with Benjamini-Hochberg
810 correction.

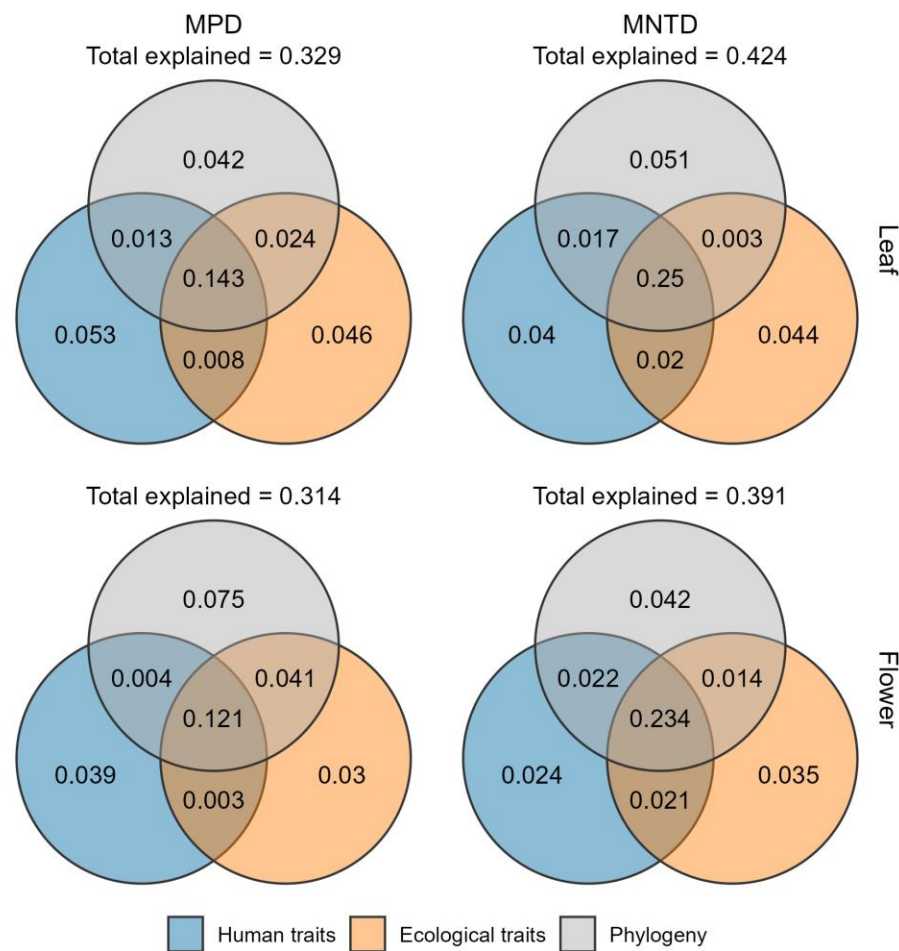


Figure S5. Venn diagrams of variation partitioning showing the relative contributions of human-associated traits (Human traits), broad ecological traits (ecological traits), and phylogenetic composition (Phylogeny) to variation in metabolite profiles for leaf-associated metabolites (left) and flower-associated volatile compounds (right). Values within intersections represent adjusted R^2 values for unique and shared explanatory fractions, while values associated with each predictor set indicate their total adjusted explanatory power.

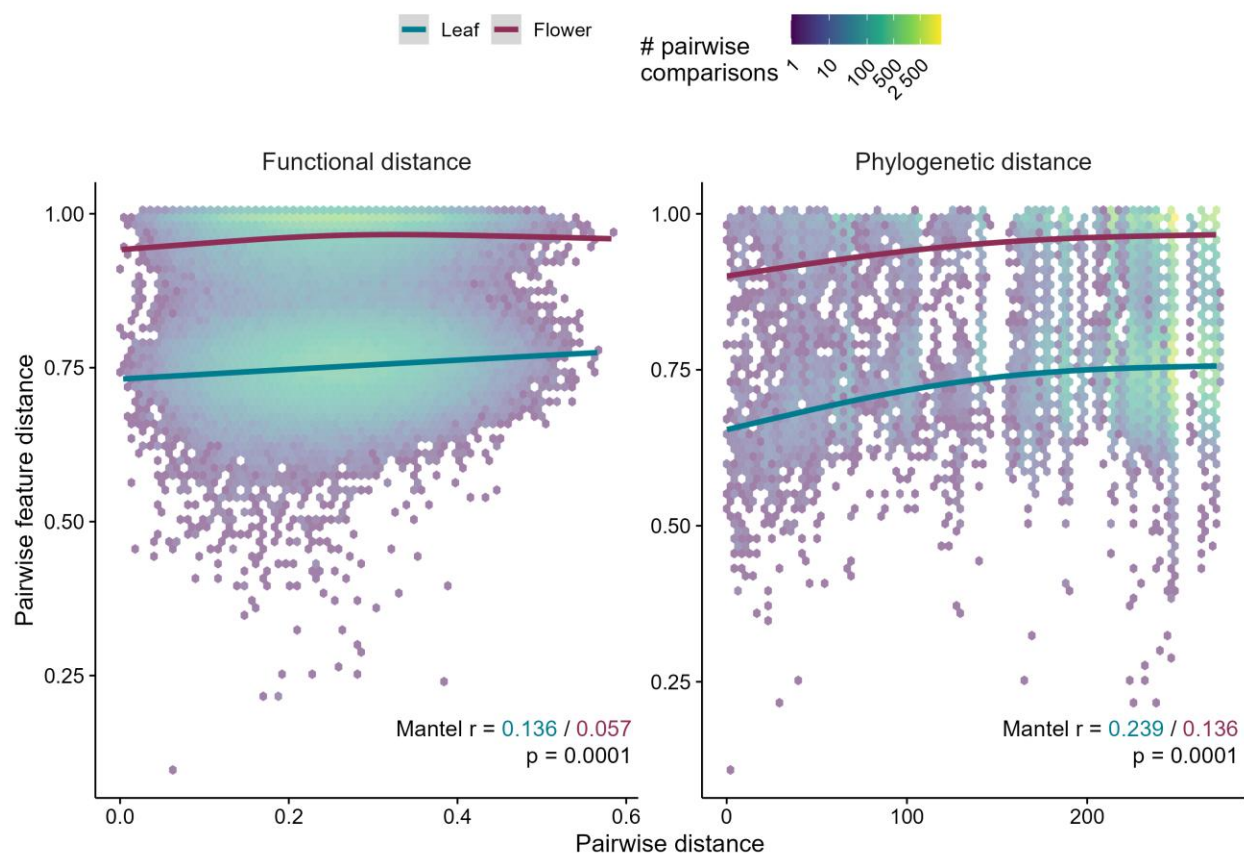


Figure S6. Relationships between pairwise functional (left) and phylogenetic (right) distances among plant species and chemical feature dissimilarity for leaf- and flower-associated metabolites. Hexagons represent the density of pairwise species comparisons, with darker shading indicating more observations. Curves show generalized additive model (GAM) fits with 95% confidence intervals for leaf (green) and flower (purple) datasets. Insets report Mantel correlation coefficients (r) and permutation test P values assessing the correspondence between chemical feature dissimilarity and phylogenetic or functional distances for each tissue.

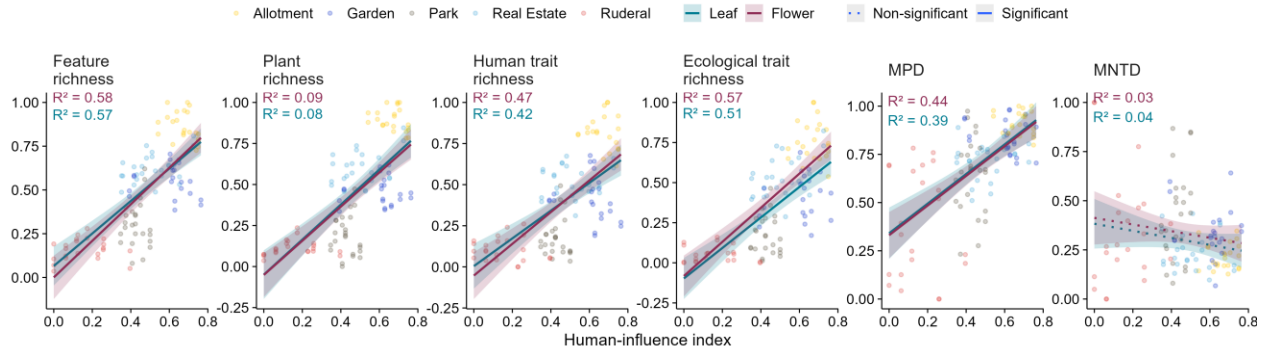


Figure S7. Relationships between the human-influence index and chemical, taxonomic, functional, and phylogenetic diversity metrics (scaled 0–1) of leaf and flower assemblages (color-coded). Points represent individual sampling sites, with regression lines showing relationships between human influence and each response variable. R^2 values and significance levels are derived from linear models. MPD = mean pairwise distance; MNTD = mean nearest taxon distance.

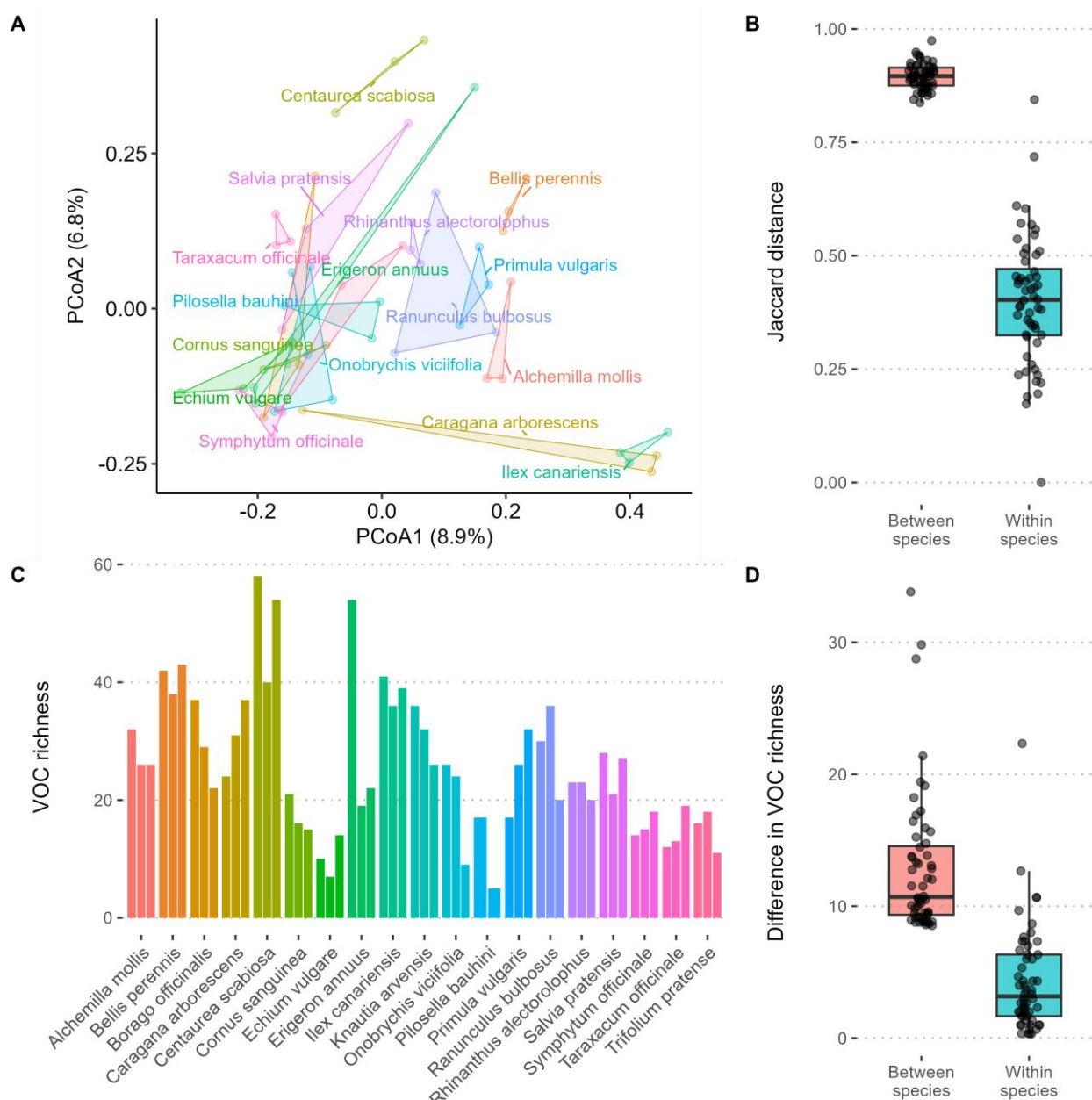
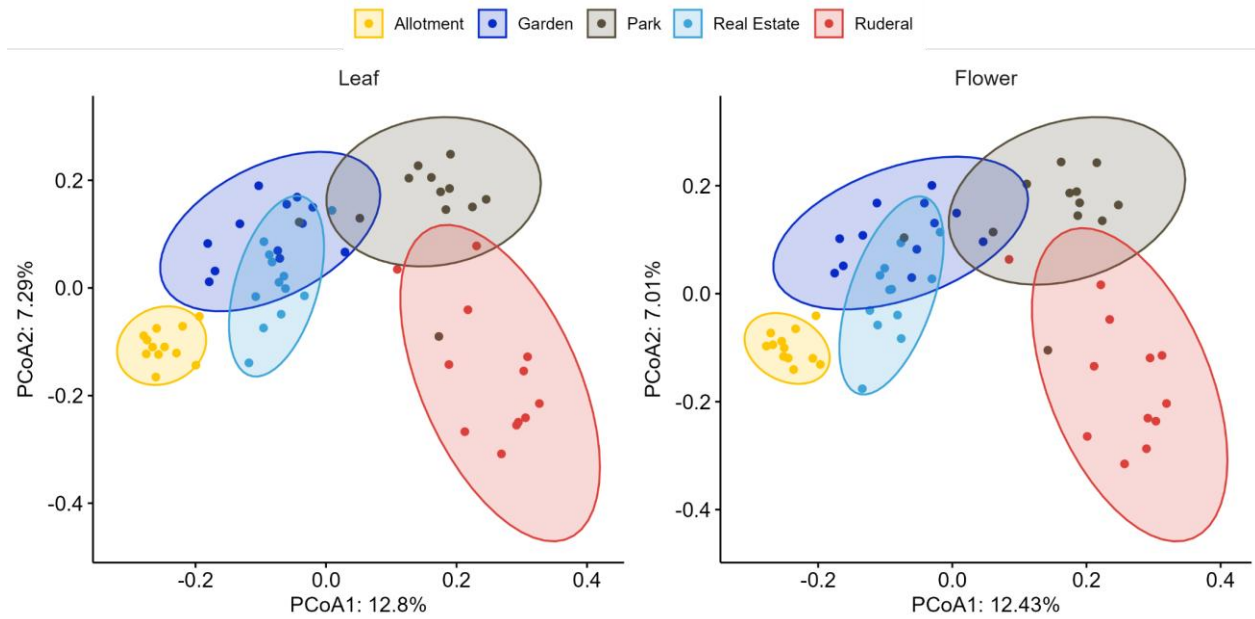


Figure S8. Species-level variation in floral VOC composition and richness. (A) principal coordinate analysis (PCoA) ordination of individual flower-associated metabolite profiles based on Jaccard dissimilarities. Points represent samples and polygons represent species-level convex hulls. (B) Distribution of metabolite compositional distances within and between plant species. (C) metabolite richness across replicated species. (D) Relative variation in metabolite richness within and between species, expressed as deviation from species-specific or among-species mean richness. Points indicate individual samples.



837 **Figure S9.** Principal coordinates analysis (PCoA) of plant species composition across UGS types
 838 (color-coded) for plant communities sampled for their leaf (left) and flower (right) metabolites.
 839 Points represent individual sites, with ellipses indicating 95% confidence intervals.

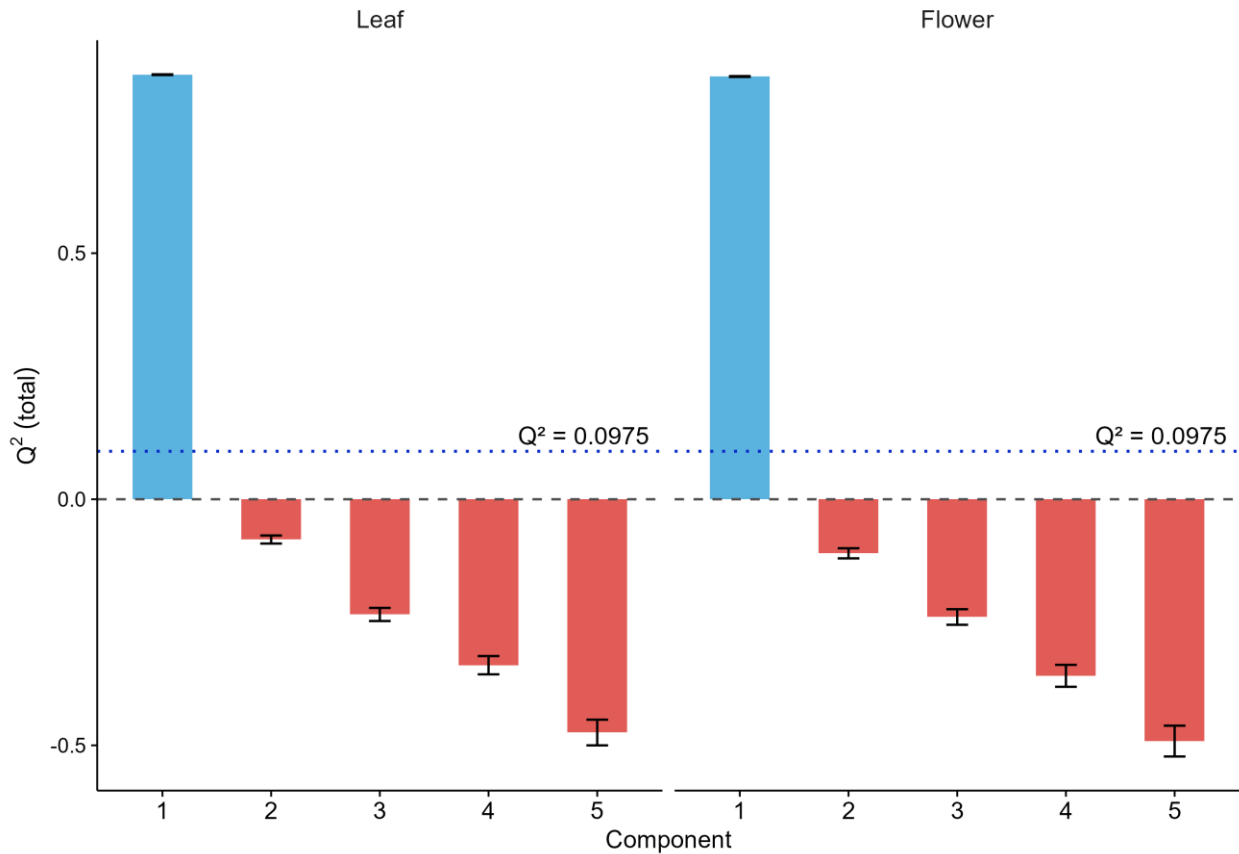


Figure S10. Predictive performance of partial least squares (PLS) regression models linking plant community-weighted functional traits to chemical feature composition across UGS. Bars show mean total Q^2 for each of five model components, with error bars representing SD from 5-fold cross-validation repeated 100 times, separately for leaf and flower tissues. Positive Q^2 values indicate predictive performance above the cross-validation baseline. The dotted line marks the commonly used Q^2 threshold of 0.0975.

846 **Table S1.** List of the 26 traits used in the analysis, based on data extracted by Grothe et al. ¹. For each trait, the table provides the source
847 dataset(s), possible trait levels, a brief description, classification as human-selected (TRUE) or not (FALSE), and references supporting
848 this classification. Further details on trait selection and data extraction are available in Grothe et al. ¹.

Trait	Dataset	Categories	Description	Human selected	Note	Source
Temperature	FloraIndicativa	alpine and nival; lower alpine, supra subalpine and upper subalpine; subalpine; lower subalpine and upper montane; montane; lower montane and upper colline; colline; warm colline; very warm colline	Characterizes the average air temperature during the growth period of a plant. It largely corresponds with the average altitudinal distribution of plants along the Alpine Arc.	FALSE		
Light	Flora-Indicativa	deep shade; shade; semi-shade; well lit places; full light	Indicates the average light quantity received in the respective habitats.	FALSE		
Moisture	FloraIndicativa	very dry; dry; moderately dry; fresh; moderately moist; moist; very moist; wet; flooded, i.e. submerged	Average soil moisture where the plant most frequently occurs.	FALSE		
Nutrients	Flora-Indicativa	very infertile; infertile; medium infertile to medium fertile; fertile; very fertile and over-rich	Nutrient content in the soil, referring mostly to nitrogen and phosphorus.	FALSE		

Humus	FloraIndicativa	little or no humus; moderate humus content; high humus content	Humus content, i.e. the totality of dead organic material in or on the soil where the plant most frequently occurs.	FALSE		
Aeration	FloraIndicativa	bad aeration; moderate aeration; good aeration	Oxygen supply of the soil where the plant most frequently occurs.	FALSE		
Growth form	TRY, BIEN, iGarten, Botanica	herb; shrub; tree; liana	Main growth form of a plant.	TRUE		Goodness, J., 2018. Urban landscaping choices and people's selection of plant traits in Cape Town, South Africa. Environmental Science & Policy 85, 182–192. https://doi.org/10.1016/j.envsci.2018.02.010
Life form	TRY, iGarten	hygrophyte; xerophyte; mesophyte; hydrophyte; chasmophyte	Describes a plants' ability to cope with special conditions regarding its substrate, water availability or nutrition strategy.	FALSE		
Annual life span	iGarten	TRUE/FALSE	Duration of a plants life cycle.	TRUE		Goodness, J., 2018. Urban landscaping choices and people's selection of plant traits in Cape Town, South Africa. Environmental Science & Policy 85, 182–192. https://doi.org/10.1016/j.envsci.2018.02.010
Flower color	TRY, BIEN, iGarten, Botanica	white; red; yellow; green; blue	Main flower color of a plant.	TRUE		Kendal, D., Williams, K.J.H., Williams, N.S.G., 2012. Plant traits link people's plant preferences to the composition of their gardens. Landscape and Urban Planning 105, 34–42. https://doi.org/10.1016/j.landurbplan.2011.11.023 Hûla, M., Flegr, J., 2016. What flowers do we like? The influence of shape and color on the rating of flower beauty. PeerJ 4, e2106. https://doi.org/10.7717/peerj.2106

Bilateral symmetry	TRY, iGarten, Botanica	TRUE/FALSE	Flower symmetry of a plant.	TRUE		Ding N, Zhong Y, Li J, Xiao Q, Zhang S, Xia H (2022) Visual preference of plant features in different living environments using eye tracking and EEG. PLoS ONE 17(12): e0279596. https://doi.org/10.1371/journal.pone.0279596 Hüla, M., Flegr, J., 2016. What flowers do we like? The influence of shape and color on the rating of flower beauty. PeerJ 4, e2106. https://doi.org/10.7717/peerj.2106
Flowering duration	FloralIndicativa	1–12	The number of months a plant usually flowers.	FALSE	The distribution of flowering periods is generally more important than the absolute duration of flowering for individual plant species (Goodness, 2018).	
Leaf greenness	TRY, iGarten	TRUE/FALSE	Leaf color of a plant. Non-green includes white, glaucous, grey, bright, red and yellow leaves.	TRUE		Kendal, D., Williams, K.J.H., Williams, N.S.G., 2012. Plant traits link people's plant preferences to the composition of their gardens. Landscape and Urban Planning 105, 34–42. https://doi.org/10.1016/j.landurbplan.2011.11.023 Goodness, J., 2018. Urban landscaping choices and people's selection of plant traits in Cape Town, South Africa. Environmental Science & Policy 85, 182–192. https://doi.org/10.1016/j.envsci.2018.02.010
Leaf ellipticness	TRY, iGarten, Botanica	TRUE/FALSE	Leaf shape/type of a plant.	TRUE		Ding N, Zhong Y, Li J, Xiao Q, Zhang S, Xia H (2022) Visual preference of plant features in different living environments using eye tracking and EEG. PLoS ONE 17(12): e0279596. https://doi.org/10.1371/journal.pone.0279596 Zhao, J., Xu, W., Li, R., 2017. Visual preference of trees: The effects of tree attributes and seasons. Urban Forestry & Urban Greening 25, 19–25. https://doi.org/10.1016/j.ufug.2017.04.015

Leaf compoundness	TRY, iGarten	TRUE/FALSE	The overall arrangement of leaves in a plant. Simple leaves are a single unit and are not divided into leaflets.	TRUE		Ding N, Zhong Y, Li J, Xiao Q, Zhang S, Xia H (2022) Visual preference of plant features in different living environments using eye tracking and EEG. PLoS ONE 17(12): e0279596. https://doi.org/10.1371/journal.pone.0279596 Zhao, J., Xu, W., Li, R., 2017. Visual preference of trees: The effects of tree attributes and seasons. Urban Forestry & Urban Greening 25, 19–25. https://doi.org/10.1016/j.ufug.2017.04.015
Leaf deciduousness	TRY, iGarten, FloraIndicativa, Botanica	TRUE/FALSE	A plants seasonal patterns of leaf development.	TRUE		Goodness, J., 2018. Urban landscaping choices and people's selection of plant traits in Cape Town, South Africa. Environmental Science & Policy 85, 182–192. https://doi.org/10.1016/j.envsci.2018.02.010 Zhao, J., Xu, W., Li, R., 2017. Visual preference of trees: The effects of tree attributes and seasons. Urban Forestry & Urban Greening 25, 19–25. https://doi.org/10.1016/j.ufug.2017.04.015
Fall conspicuousness	TRY, iGarten	TRUE/FALSE	Whether a plants foliage is conspicuous (i.e. prominent) in fall.	TRUE		Xu, W., Jiang, B., Zhao, J., 2022. Effects of seasonality on visual aesthetic preference. Landscape Research 47, 388–399. https://doi.org/10.1080/01426397.2022.2039110 Zhao, J., Xu, W., Li, R., 2017. Visual preference of trees: The effects of tree attributes and seasons. Urban Forestry & Urban Greening 25, 19–25. https://doi.org/10.1016/j.ufug.2017.04.015
CRS competitive	FloraIndicativa	TRUE/FALSE	Whether a plant is considered competitive according to Grime (1979, 2001). Note that most plants cannot be distinctly categorized into one of the three primary strategy groups, therefore this trait is multilabel (i.e., a plant can have a 1 in more than one of these CRS traits).	FALSE		
CRS stress-tolerant	FloraIndicativa	TRUE/FALSE	Whether a plant is considered stress-tolerant according to Grime (1979, 2001). Stress-tolerant strategists are adapted to harsh environmental conditions. In most cases, plants are small and slow-growing, having small and often evergreen leaves.	FALSE		
CRS ruderal	FloraIndicativa	TRUE/FALSE	Whether a plant is considered ruderal according to Grime (1979, 2001). Ruderal strategists are short-lived, small, light-demanding pioneer plants that are rarely woody and produce a large amount of seeds that are able to rapidly spread.	FALSE		

Plant height vegetative	TRY, BIEN, iGarten, Botanica	meters	Central to a species carbon gain strategy because height is a major determinant of a plant's ability to compete for light. Strongly correlated with life span and seed mass. Low plant height is often associated with adaptations to shade and resource conservation, while high plant height indicates adaptations for light competition and dispersal.	TRUE		Goodness, J., 2018. Urban landscaping choices and people's selection of plant traits in Cape Town, South Africa. <i>Environmental Science & Policy</i> 85, 182–192. https://doi.org/10.1016/j.envsci.2018.02.010 Zhao, J., Xu, W., Li, R., 2017. Visual preference of trees: The effects of tree attributes and seasons. <i>Urban Forestry & Urban Greening</i> 25, 19–25. https://doi.org/10.1016/j.ufug.2017.04.015
SLA	TRY, BIEN	millimeters ² /milligrams	SLA = Specific Leaf Area; Ratio of leaf area to leaf dry mass, i.e. how much leaf area a plant builds with a given amount of biomass. Reflects the trade-off between resource capture (i.e., leaf area) and resource conservation (i.e., biomass). High SLA values are associated with “fast-return” strategies, where plants allocate resources to maximize photosynthetic efficiency and rapid growth. Low SLA values are associated with “slow-return” strategies, where plants invest resources in durable tissues and long-term persistence.	FALSE		
Leaf water content per leaf dry mass	TRY	grams (water)/grams (dry mass)	Ratio of leaf water content to leaf dry mass. Reflects the hydration status of leaf tissues and the ability of plants to regulate water balance. Can indicate adaptations to water-limited environments.	FALSE		
LDMC	TRY, BIEN	grams /grams	LDMC = Leaf Dry Matter Content; Ratio of leaf dry mass to leaf fresh mass. Reflects the density and thickness of leaf tissues and the allocation of resources within leaves. High LDMC suggests a high proportion of dry matter in relation to the total leaf mass, which typically corresponds to thicker leaves with denser tissues. Thicker leaves with higher LDMC values often have denser cell walls and more structural reinforcement, making them less susceptible to herbivory. Conversely, low LDMC values indicate a lower proportion of dry matter in relation to the total leaf mass, which corresponds to thinner leaves with less structural density. These thinner leaves typically have higher SLA, meaning they have a higher surface area-to-mass ratio, and are often associated with rapid growth and resource acquisition strategies.	FALSE		

Seed dry mass	TRY, BIEN	milligrams	Reflects investment in reproductive effort, which may strongly influence seed dispersal, seedling growth, resource assimilation capacity, and competitive and reproductive ability once a plant is established. Small seed mass is often associated with high reproductive output and opportunistic colonization, while high seed mass indicates investment in offspring quality rather than quantity.	FALSE		
Non-native	Inflorescence	TRUE/FALSE	Indicates whether a species is considered alien in Switzerland.	TRUE		Kendal, D., Williams, K.J.H., Williams, N.S.G., 2012. Plant traits link people's plant preferences to the composition of their gardens. Landscape and Urban Planning 105, 34–42. https://doi.org/10.1016/j.landurbplan.2011.11.023

849

850 **Reference:**

851 1. Grothe, V., Dädlow, G.M.L., Casanelles, J., Ruile, S., Moretti, M., Fournier, B., 2026. The Human-Imprinted Regional Species

852 Pool: Functional Trait Patterns of Commercial and Established Plants. Authorea. <https://doi.org/10.22541/authorea.15003231/v1>

Table S2: Goodness-of-fit statistics for the structural equation models (SEM) evaluating relationships between the human-influence index and functional, phylogenetic, and chemical diversity metrics for leaf- and flower-associated metabolites. Fit was evaluated using Fisher's C and Chi-squared tests, with corresponding values, p-values, and degrees of freedom (df) reported for each model.

	<i>Metric</i>	<i>Value</i>	<i>p-value</i>	<i>df</i>
<i>Leaf</i>	<i>Chi-Squared</i>	<i>0.928</i>	<i>0.335</i>	<i>1</i>
	<i>Fisher's C</i>	<i>2.070</i>	<i>0.355</i>	<i>2</i>
<i>Flower</i>	<i>Chi-Squared</i>	<i>1.065</i>	<i>0.302</i>	<i>1</i>
	<i>Fisher's C</i>	<i>2.267</i>	<i>0.322</i>	<i>2</i>

Table S3: Independence claims tested within structural equation models (SEMs) evaluating relationships between the human-influence index and functional, phylogenetic, and chemical diversity metrics for leaf- and flower-associated metabolites. Each claim represents a hypothesized absence of a direct relationship between variables implied by the model structure. For each model, critical values, p-values, and degrees of freedom (df) are reported to assess whether independence assumptions are supported based on standard significance thresholds.

	<i>Independence claim</i>	<i>Critical value</i>	<i>p-value</i>	<i>df</i>
<i>Leaf</i>	<i>MNTD ~ human_index</i>	<i>0.933</i>	<i>0.355</i>	<i>53</i>
<i>Flower</i>	<i>MNTD ~ human_index</i>	<i>1.000</i>	<i>0.322</i>	<i>53</i>

866 *Supplementary Material I*

867 To assess intraspecific variation in flower-associated metabolite profiles, we sampled three
868 individuals from 19 of the most commonly encountered species and analyzed them using the same
869 workflow as all other samples (see *Flower volatile organic compounds*). We evaluated
870 compositional variation among replicates using Principal Coordinate Analysis (PCoA) based on
871 Jaccard dissimilarities (Fig. S10A). We then compared within- and between-species variation by
872 calculating the distance of each replicate to the centroid of its respective species and to the centroids
873 of all other species (Fig. S10B). Finally, we assessed variation in metabolite richness by comparing
874 the number of detected features per sample (Fig. S10C) and quantifying deviations from the
875 species-specific mean richness within and among species (Fig. S10D).

877 Plant and chemical diversity relationships were quantified separately for leaf- and flower-
878 associated datasets. Differences in chemical feature richness among habitat types were evaluated
879 using pairwise Wilcoxon rank-sum tests with Benjamini–Hochberg correction. To assess whether
880 variation in chemical richness was associated with plant diversity and whether the strength of this
881 relationship varied with UGS type, we then fitted negative binomial generalized linear models
882 separately for each tissue type and habitat category, with chemical feature richness as the response
883 variable and plant species richness as the explanatory variable. Model coefficients were extracted
884 to estimate the strength and direction of the relationship between plant and chemical richness, while
885 model performance was assessed using a pseudo- R^2 calculated from the proportional reduction in
886 deviance relative to the corresponding null model.

888 We reconstructed a species-level phylogeny using the extended GBOTB mega-tree implemented
889 in V.PhyloMaker2⁵⁷, providing a phylogenetic framework for the flowering-plant species included
890 in each dataset. Species were placed into the reference phylogeny using phylo.maker with scenario
891 S3 (all scenarios producing the same results). Phylogenetic relationships were quantified from
892 branch lengths by calculating a cophenetic distance matrix, with each pairwise distance
893 representing the evolutionary path length separating two species. This matrix was combined with
894 presence-absence community matrices to quantify within-community phylogenetic structure using
895 two complementary metrics: mean pairwise distance (MPD), the mean phylogenetic distance
896 among all species pairs within a site, and mean nearest taxon distance (MNTD), the mean distance
897 from each species to its closest relative within the community. MPD captures the overall breadth
898 of evolutionary lineages represented and is more sensitive to turnover among distantly related taxa,
899 whereas MNTD emphasizes terminal phylogenetic structure and is more sensitive to turnover
900 among closely related species. The same MPD/MNTD framework was used to quantify
901 phylogenetic turnover among sites, capturing broad- and fine-scale differences in community
902 composition.

903 Functional composition was quantified using the mFD framework⁶¹ based on Gower distances,
904 integrating continuous, ordinal, binary and categorical traits with equal weighting, to measure
905 dissimilarities between species. The resulting species-by-species functional distance matrix was
906 summarized using PCoAs to represent species in a reduced multidimensional functional space. The
907 number of PCoA axes was selected using the mean absolute deviation (MAD) criterion, retaining
908 the dimensionality that minimized MAD, with a minimum of two and maximum of six axes.
909 Functional turnover among sites was then quantified using the same MPD/MNTD framework,

910 capturing broad- and fine-scale shifts in trait composition. Because average pairwise trait distances
911 do not directly quantify the extent or distribution of occupied functional space, within-community
912 functional diversity was additionally quantified from the PCoA space using functional richness
913 (FRic) and functional dispersion (FDis), two common functional diversity metrics. FRic measures
914 the volume of multidimensional functional space occupied by species in a community, whereas
915 FDis measures the occurrence-weighted distance of species from the community functional
916 centroid. FRic and FDis were calculated separately for human-associated traits and the broader set
917 of ecological traits.