

Phylogenetic, allometric, and functional group structure in chemical sensitivity across aquatic taxa

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Abstract

Chemical risk assessment across diverse communities remains challenging because most chemical-species pairs are empirically untested. Identifying phylogenetic, allometric, and functional group structure in chemical sensitivity may support cross-species extrapolation and community risk assessment, yet how these factors explain sensitivity across diverse taxa and chemicals remains poorly understood. We examined how phylogenetic relatedness, body mass, and functional group shape relative sensitivity across 580 aquatic species and 1103 chemicals spanning six chemical-use groups. We quantified phylogenetic signal in species relative sensitivity and fitted Bayesian phylogenetic hierarchical models to test global allometry, functional group-specific baseline sensitivity, and functional group-specific allometry. Phylogenetic signal was strong in invertebrates but weak in algae and fish. Models allowing both baselines and slopes to vary among functional groups received the strongest predictive performance across all taxonomic and chemical-use group combinations. However, most standardised slopes were weak, with moderate allometric effects concentrated in a few functional groups. Fixed effects explained only a modest proportion of variation, whereas chemical identity and phylogenetic structure captured substantial additional variation, with phylogeny dominating. These findings reveal limited support for general allometric rules and provide a basis for integrating functional group and phylogenetic information into cross-species extrapolation and higher-tier chemical risk assessment.

Keywords

Aquatic ecotoxicology, chemical sensitivity, allometry, phylogeny, functional groups, chemical risk assessment, cross-species extrapolation

1. Introduction

Contamination of the environment with diverse compounds, such as pesticides, pharmaceuticals and metals, has become a major environmental challenge¹. Chemical pollution affects organisms across multiple levels of biological organisation, from individual physiology to community structure and functioning, ultimately influencing biodiversity and ecosystem processes^{2,3}. Consequently, there is increasing interest in higher-tier chemical risk assessment, which moves beyond traditional single-species toxicity tests to consider species diversity, ecological interactions, and responses at higher levels of biological organisation^{4,5}. This shift highlights the need for predictive ecotoxicology: approaches that can infer chemical sensitivity across species from shared biological characteristics, including their traits and evolutionary relationships. Such predictive approaches are particularly important because empirical toxicity data are available for only a small subset of possible species-chemical combinations, leaving the sensitivity of most species to most chemicals unknown⁶.

Identifying general principles that link variation in species chemical sensitivity to the trait-based structure of ecological communities may provide a bridge^{7,8}. In risk assessment based on food webs and delivering information on endpoints such as biodiversity change and ecosystem function, species-level sensitivity determines which nodes are directly affected by chemical exposure, while trophic interactions determine how these toxicity effects propagate through communities^{9–11}. Species sensitivities are unlikely to be randomly distributed across communities and chemicals¹². Organisms share evolutionary histories, physiological and functional traits that may generate biologically structured patterns in sensitivity to chemicals^{13,14}. Furthermore, within food webs, species can be categorized into trophic guilds and/or functional groups that share similar resources and consumers. Key bioenergetic rates in these species scale allometrically, with body mass as a master trait that shapes growth, metabolism, and predation^{15–17}. Given that species sensitivity to chemicals is also expected to be mediated by size-dependent toxicokinetics and toxicodynamics processes, including uptake, biotransformation, and the balance between internal dose and organismal turnover^{14,18,19}, sensitivity may scale systematically with body mass.

Consistent with this expectation, several studies have reported clear allometric dependence in sensitivity, including terrestrial vertebrates exposed to various chemicals^{20–22}, bees exposed to insecticides²³, freshwater fish exposed to cadmium²⁴, aquatic insects exposed to metals²⁵, and stream amphipods exposed to micropollutants²⁶. Evidence for size dependence has also been linked to body size-dependent toxicokinetics and toxicodynamics¹⁹ and pharmacokinetic parameters²⁷. Other analyses, however, find weak allometric effects^{28–30}. These studies not only deliver equivocal insight but they also share a common limitation of focussing on a narrow range of taxa or chemicals. Together, this highlights the need for a more taxonomically and chemically diverse assessment of when and why allometric relationships hold.

Functional groups may provide an important axis for understanding variation in chemical sensitivity. Although direct tests of sensitivity differences among functional groups remain limited, trait-based ecotoxicological studies suggest that feeding habits can help explain interspecific variation in chemical responses, particularly among invertebrates^{14,18,28,31}. Thus, even species with similar body mass may still differ in sensitivity if they belong to different functional groups. Community-level studies also support this and show that functional composition of communities can shape contaminant responses. For example, heavy metal effects in invertebrate communities have been linked to the relative abundance of predators³².

Such trait-based analyses must account for phylogenetic non-independence among species³³. Body mass and functional groups both show phylogenetic structure^{34,35}, and chemical sensitivity itself may also exhibit phylogenetic structure, such that closely related species display similar sensitivities because they share evolutionary history, such as through conserved molecular targets, physiological pathways, or detoxification mechanisms^{6,14,36}. Consequently, observed relationships between traits and sensitivity may partly reflect shared ancestry rather than causal trait effects, resulting in residual similarity beyond body mass and functional groups. Phylogenetic correction is thus needed to prevent pseudo-replication and to test whether and how body mass and functional groups explain sensitivity beyond shared ancestry.

Despite its importance, evidence of phylogenetic structure in chemical sensitivity remains inconsistent. Most previous tests of body size-sensitivity relationships have not explicitly accounted for phylogeny, with few exceptions³⁷, which reported that allometric patterns weakened after incorporating phylogenetic relatedness. Evidence for phylogenetic signals in sensitivity is likewise mixed. For example, stronger signals have been observed for particular chemical classes such as organophosphates in fishes³⁸, and in amphibians for some insecticides³⁹ and for copper sulfate⁴⁰. However, signals were also reported generally low in fishes³⁷ and detected for only a minority of chemicals across aquatic taxa⁴¹. Moreover, existing analyses are often limited in taxonomic or chemical coverage, preventing a unified assessment across the tree of life.

In this study, we examined how phylogenetic relatedness, body mass, and functional group explain variation in chemical sensitivity across 580 aquatic species spanning algae, invertebrates, and fish, using sensitivity estimates for 1103 chemicals across six chemical-use groups: industrial chemicals, pharmaceuticals, and pesticides targeting arthropods, plants, microbes, or mixed targets. By integrating these sensitivity data with genus-level phylogeny, species body mass, and functional group classification, we tested whether chemical sensitivity is structured primarily by shared evolutionary history, by a common allometric relationship with body mass, by functional group differences in baseline sensitivity, or by functional group-specific allometric scaling (**Figure 1**). Together, our model evaluations test whether species sensitivity follows general allometric rules or instead depends on functional group, evolutionary relatedness, and chemical-use

context. By identifying these sources of variation, this study provides trait- and phylogeny-informed insights to support future community, especially food web risk assessment.

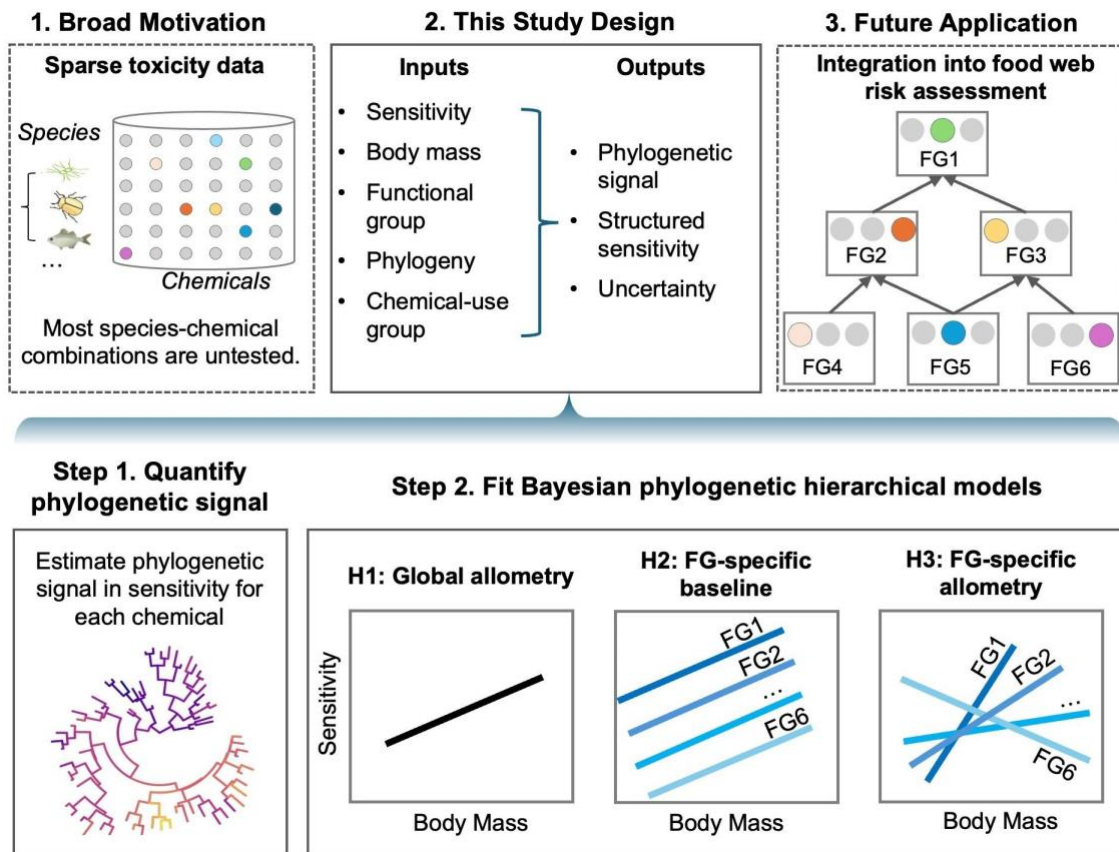


Figure 1. Conceptual framework for analysing phylogenetic, allometric, and functional group structure in species chemical sensitivity. Sparse toxicity tests leave many species and chemical combinations unmeasured. Trait- and phylogeny-informed insights offer one way to describe structured variation in species sensitivity and may support future integration into food web risk assessment. In this study, we combine relative sensitivity data with body mass, functional group (FG), and phylogeny. First, we quantify phylogenetic signal in species relative sensitivity within each taxonomic group and chemical-use group. Second, we use hierarchical Bayesian regression models with explicit phylogenetic random effects to compare three hypotheses: H1, global allometry, in which species share a common body-mass scaling relationship; H2, FG baselines, in which FGs differ in baseline sensitivity but share a common body mass slope; and H3, FG allometry, in which FGs differ in both baseline sensitivity and body mass scaling. These analyses identify whether species sensitivity is structured by evolutionary relatedness, body mass, and functional groups.

2. Methods

2.1 Species chemical sensitivity

2.1.1 Sensitivity data assembly and prediction

We assembled observed toxicity data from three sources. First, we used the ADORE dataset⁴², which reports LC₅₀ or EC₅₀ values at four standard exposure durations (24, 48, 72, and 96 h). After harmonising species names and taxonomy using the GBIF Backbone Taxonomy through the *rgbif* R package version 3.8.3, accessed in April 2026, we retained data for 1155 species of algae, crustaceans, and fish tested against 3289 chemicals, comprising 18451 unique species-chemical pairs. To expand coverage of non-crustacean invertebrates, particularly insects and molluscs, we added LC₅₀ data for exposure to metals and insecticides^{43,44}. These studies assembled toxicity records from the US EPA ECOTOX database and the literature. These records were harmonised with ADORE by retaining only aquatic experiments with static, flow-through, renewal, or unreported exposure types (ECOTOX definitions), freshwater or saltwater media, exposure durations of 24, 48, 72, or 96 h, and mortality endpoints. This addition contributed 231 species, 38 chemicals, and 533 observed species-chemical combinations. The combined observed sensitivity dataset comprised 1376 unique species (766 genera), 3289 chemicals, and 18974 unique species-chemical pairs.

We then used the pairwise machine-learning model developed by Posthuma et al.⁴⁵ to predict sensitivity for all species-chemical-duration combinations. We followed the published workflow (https://github.com/rivm-syso/adore_pairwise_learning/) and incorporated the expanded observed toxicity dataset described above. The model showed good predictive performance (**Figure S1**), with an adjusted R² of 0.74 and an RMSE of 0.84 on the log₁₀ concentration scale. These values were similar to those reported by Posthuma et al.⁴⁵, indicating that expanding the dataset to include additional non-crustacean invertebrates did not compromise the model's overall predictive performance. The model generated predicted sensitivity estimates for all combinations of 1376 species, 3289 chemicals, and four exposure durations (**Figure S2**). For subsequent analyses, we used 72 h estimates for algae and 96 h estimates for invertebrates and fish, corresponding to the standard durations most commonly used for these taxonomic groups.

To quantify interspecific variation in sensitivity within each chemical, we expressed each species' sensitivity relative to the sensitivity of *Daphnia magna*, a widely used reference organism, to the same chemical⁴⁶. This chemical-specific normalisation provided a consistent reference against which differences among species could be evaluated, thereby facilitating the characterisation of relative sensitivity patterns and their associations with body mass, functional group, and phylogenetic relatedness.

2.1.2 Chemical-use groups

We assigned each of the 3289 chemicals in our dataset to a primary use category by matching them with the classifications from Kramer et al⁴⁷ and the online Pesticide Properties Database (PPDB⁴⁸). For chemicals matched to the PPDB, classifications were based, where available, on the Pesticide type field under General status. Based on the available chemical-use information, 1103 chemicals were classified into six chemical use groups: industrial chemicals (215), pharmaceuticals (121), and pesticides, which were further subdivided into targeting arthropods (202), plants (333), microbes (136), and mixed target (96) categories. Chemicals without explicit use assignments were excluded from downstream analyses. Throughout, we summarise relative sensitivity across all chemicals within each chemical-use group using medians and interquartile ranges (IQRs), with the lower and upper IQR bounds corresponding to the 25th and 75th percentiles, respectively.

2.2 Species phylogeny, body mass, and functional groups

We reconstructed a genus-level phylogeny using the *rotl* R package version 3.1.0⁴⁹, with taxon names matched to Open Tree Taxonomy version 3.7. Taxa that could not be resolved to species level were excluded, and retained species were represented by their corresponding genera in the phylogeny. We assigned branch lengths using the Grafen method, and derived the phylogenetic variance-covariance matrix using the *ape* R package⁵⁰ to account for shared evolutionary history in subsequent analyses. In total, 871 species across 553 genera were placed in the phylogeny.

For species included in the phylogeny, we assembled body mass data for 599 species across 332 genera from the literature and public datasets. When multiple measurements were available within or across sources, we used the average value. If species-level data were unavailable, we used the genus-level mean calculated from all species in the same genus for which body mass data were available.

Next, we assigned species to functional groups commonly used in food web structure and modelling. Algal species were assigned to three functional resource groups – diatoms, green algae, and other algae comprising chrysophytes, cryptomonads, dinoflagellates, haptophytes, and stramenopiles. Invertebrate species were assigned to five functional groups – filterers, gatherers, shredders, herbivores, and predators (**Table S1**). Because one focal chemical group targets arthropods, we further split invertebrate functional groups into arthropod functional groups or non-arthropod functional groups (e.g., arthropod filterers vs non-arthropod filterers). Non-arthropod shredder taxa were absent in the final dataset. Fish species were assigned to trophic guilds based on adult diet composition from FishBase and literature. Six trophic guilds were specified: detritivore, planktivore, herbivore, invertivore, omnivore, and piscivore. Detritivore and herbivore were merged due to overlap and small sample sizes, and the parasitic guild was

excluded as only one single species was present in the final dataset. All species-level body mass data and functional group assignments, together with their original sources, are provided in the archived dataset⁵¹.

The final dataset comprised 580 species from 320 genera and 1103 chemicals. This included 79 algal species from 45 genera, 336 invertebrate species from 173 genera, and 165 fish species from 102 genera. Detailed sample sizes across chemical-use and functional groups are provided in **Table S2**.

2.3 Statistical analysis

2.3.1 Phylogenetic signal

We quantified phylogenetic signal in species relative sensitivity using Pagel's λ , which measures the extent to which trait covariance among taxa follows the expectation from shared evolutionary history under a Brownian-motion model^{33,52}. Values close to 0 indicate little or no phylogenetic signal, whereas values close to 1 indicate covariance approaching the Brownian-motion expectation.

Because the phylogenies were resolved at the genus level, chemical sensitivity was first aggregated by genus and chemical identity by calculating the mean $\log_{10}$ relative sensitivity for each genus exposed to each chemical. Pagel's λ was then estimated separately for each chemical within each taxonomic group. Pagel's λ and its significance were estimated using the *phylosig* function in the *phytools* package in R⁵³, with likelihood-ratio tests assessing whether λ differed from zero. *P* values were adjusted within each taxon and chemical-use group combination using the Benjamini–Hochberg procedure.

To test whether phylogenetic signals differed among taxonomic and chemical-use groups, chemical-specific λ estimates were compared using a two-way ANOVA with taxonomic group, chemical-use group, and their interaction as explanatory factors. Post-hoc pairwise comparisons among chemical-use groups within each taxonomic group were performed using estimated marginal means, with Benjamini–Hochberg correction applied separately within each taxonomic group.

2.3.2 Bayesian phylogenetic hierarchical models

We used Bayesian phylogenetic hierarchical models to test three alternative hypotheses for how body mass and functional group explain variation in species relative sensitivity, while accounting for chemical identity and phylogenetic relatedness (**Figure 1**). These hypotheses were tested separately within each taxonomic group and chemical-use group combination. This stratification was used because chemical-use groups differ in intended targets, modes of action, and taxonomic

selectivity, and because algae, invertebrates, and fish are separated by deep evolutionary divergences that make a single global phylogenetic model difficult to justify and interpret biologically.

For each combination of taxonomic group and chemical-use group, we fitted four candidate models that shared the same random-effect structure but differed in their fixed effects (**Table 1**). The null model M0 contained no fixed predictors. Model M1 included body mass, testing for a common allometric relationship in sensitivity. Model M2 included body mass and functional group as additive fixed effects, allowing functional groups to differ in baseline sensitivity while sharing a common body-mass slope. Model M3 included an interaction between body mass and functional group, allowing both baseline sensitivity and body-mass slopes to differ among functional groups.

Table 1. Summary of Bayesian phylogenetic hierarchical models used to test hypotheses of species relative sensitivity. Sensitivity and Mass denote standardised $\log_{10}$ relative sensitivity and body mass, respectively; σ_{chemical} denotes a random intercept for chemical identity. σ_{phylo} denotes a phylogenetic random effect incorporating the genus-level phylogenetic covariance matrix.

Model	Structure	Hypothesis tested
M0	$\text{Sensitivity} \sim \sigma_{\text{chemical}} + \sigma_{\text{phylo}}$	H0: Null model.
M1	$\text{Sensitivity} \sim \text{Mass} + \sigma_{\text{chemical}} + \sigma_{\text{phylo}}$	H1: Global allometry. Sensitivity follows a common body-mass scaling relationship.
M2	$\text{Sensitivity} \sim \text{Mass} + \text{FGs} + \sigma_{\text{chemical}} + \sigma_{\text{phylo}}$	H2: Group baselines. Functional groups (FGs) differ in baseline sensitivity, while sharing a global body-mass scaling relationship.
M3	$\text{Sensitivity} \sim \text{Mass} * \text{FGs} + \sigma_{\text{chemical}} + \sigma_{\text{phylo}}$	H3: Group allometry. Both baseline sensitivity and body-mass scaling relationships differ among functional groups.

Species relative sensitivity and body mass were $\log_{10}$ -transformed and then standardised to zero mean and unit variance within each combination of taxonomic group and chemical-use group. Slopes therefore represent changes in standardised sensitivity per standard deviation increase in $\log_{10}$ body mass, and functional group intercepts describe baseline sensitivity at the corresponding dataset's mean $\log_{10}$ body mass. All models included crossed random effects for chemical identity and genus. Each combination of species and chemical was represented by a single observation, so there were no replicates at this level. However, observations involving the same chemical shared a chemical-specific intercept, while observations belonging to the same genus shared a genus-level effect, with effects for different genera correlated according to their phylogenetic relatedness. The genus-level effect was assumed to be consistent across individual chemicals within each fitted dataset.

Models were implemented using the *brms* package in R⁵⁴, utilising the Stan probabilistic programming language via the *cmdstanr* backend. All models used a Gaussian likelihood with an identity link. We specified common regularising priors across taxonomic and chemical-use groups. Fixed-effect coefficients, including functional group intercepts and body-mass slopes, were assigned Normal(0, 0.5) priors. Chemical and phylogenetic random-effect standard deviations were assigned Exponential(1) and half-normal(0, 1.5) priors, respectively. The residual standard deviation was assigned a half-Student-t(3, 0, 0.5) prior. For each model, we ran four Markov chain Monte Carlo chains with 8000 iterations per chain, including 4000 warm-up iterations, yielding 16000 post-warm-up posterior samples in total. Model convergence was assessed using the potential scale reduction statistic ($R\text{-hat} < 1.01$) and by ensuring sufficient effective sample sizes for all parameters⁵⁵ (**Table S3**). Model adequacy was evaluated using posterior predictive checks (Figure S3).

2.3.3 Model comparison and explanatory power

Candidate models were compared separately within each taxonomic group and chemical-use group combination using approximate leave-one-out cross-validation (LOO)⁵⁶. LOO estimates how reliably a model predicts withheld observations, summarised by the expected log predictive density (ELPD). Higher ELPD indicates better predictive performance. We thus defined the model with the highest ELPD as the best-predicting model. Although models M0–M3 progressively increased in complexity, additional effects improved ELPD only when they improved prediction of withheld observations, thereby limiting support for overfitted models. Model comparison was therefore interpreted in terms of predictive support for the proposed body-mass and functional-group structures rather than as formal hypothesis testing.

For the best-supported model in each combination, we quantified model fit using marginal and conditional R^2 , representing variance explained by fixed effects alone and by both fixed and random effects, respectively. We further partitioned unexplained variation among chemical identity, phylogenetic structure, and residual variation to assess the relative contribution of chemical heterogeneity, shared evolutionary history, and unexplained species-level variation to patterns of chemical sensitivity.

2.3.4 Posterior effect size and pairwise contrasts

Given that the group-specific allometry model was the best-supported model for each taxonomic group and chemical-use group combination (cf. Figure 4), we quantified allometric effect sizes using its posterior standardised slopes (β_{std}) and pairwise contrasts to evaluate the magnitude of allometric relationships and differences among functional groups. For each functional group-specific slope, we calculated the posterior median and 95% highest density interval (HDI)⁵⁷. We assessed practical magnitude by comparing the HDI with a predefined region of practical

equivalence (ROPE) of $\pm 0.20^{57}$. This boundary corresponds to a 0.20-standard-deviation change in log10 relative sensitivity per one-standard-deviation increase in log10 body mass. Slopes with 95% HDIs entirely within the ROPE were interpreted as small effect sizes, whereas those with HDIs entirely outside the ROPE were interpreted as moderate or stronger allometric effects. Slopes whose 95% HDIs crossed a ROPE boundary were classified as uncertain because their posterior distributions included both weak and potentially meaningful body mass effects.

To compare allometric slopes among functional groups, we calculated pairwise contrasts between functional group-specific standardised slopes within each taxonomic group and chemical-use group combination. For each posterior draw, slope contrasts were calculated as the difference between two functional group-specific standardised slopes, $\Delta\beta_{\text{std}}$. Slope contrasts were then summarised using medians and 95% HDIs and evaluated against ROPE thresholds of ± 0.20 and ± 0.50 .

To compare baseline sensitivity, we calculated pairwise contrasts between functional group-specific intercepts at the corresponding dataset's mean log10 body mass. For each posterior draw, contrasts were expressed relative to the residual standard deviation as $d = \frac{\alpha_i - \alpha_j}{\sigma}$, where α_i and α_j are the functional group-specific intercepts for two functional groups, and σ is the residual standard deviation. Posterior medians and 95% HDIs were calculated for each baseline contrast. Baseline contrasts were compared with ROPE thresholds of ± 0.20 , ± 0.50 , and ± 0.80 .

All analyses were conducted in R 4.5.0⁵⁸.

2.3.5 Robustness analysis

To assess the robustness of our inferences to the inclusion of machine-learning-predicted sensitivity estimates, we repeated the phylogenetic-signal and functional group-specific allometry analyses after progressively excluding 5%, 10%, and 15% of predicted sensitivity estimates (**Appendix S1**).

3. Results

3.1 Relative sensitivity across taxa and chemical-use groups

The compiled dataset comprised 580 species from 320 genera and sensitivity estimates for 1103 chemicals classified into six chemical-use groups. To characterise broad patterns, we first calculated mean relative sensitivity for each genus-chemical combination and then summarised these estimates by taxonomic group and chemical-use group.

Relative sensitivity, expressed on a $\log_{10}$ scale, varied across taxonomic and chemical-use groups (**Figure 2**). A value of zero indicates sensitivity equal to that of the reference species, while negative and positive values indicate greater and lower sensitivity, respectively. Considerable variation in relative sensitivity occurred among species within each group, with substantial overlap in the distributions of taxonomic groups. For industrial chemicals, algae had the lowest median value and were therefore the most sensitive group (median: 0.11; IQR: -0.01 to 0.28), followed by invertebrates (0.16; 0.01 to 0.32) and fish (0.28; 0.09 to 0.42). A similar pattern was observed for pharmaceuticals, with algae showing the greatest sensitivity (0.03; -0.15 to 0.10), followed by invertebrates (0.09; -0.07 to 0.23) and fish (0.21; 0.03 to 0.37).

Taxonomic differences were most apparent for pesticides targeting plants and microbes. For pesticides targeting plants, algae showed the greatest relative sensitivity (-0.05; -0.18 to 0.13), followed by invertebrates (0.08; -0.08 to 0.23) and fish (0.23; 0.04 to 0.37). A similar pattern occurred for pesticides targeting microbes, with sensitivity decreasing from algae (0.06; -0.06 to 0.25) to invertebrates (0.13; -0.03 to 0.28) and fish (0.24; 0.07 to 0.40).

Differences among taxa were smaller for pesticides targeting arthropods and mixed-target pesticides, with substantial overlap in relative sensitivity distributions. For pesticides targeting arthropods, invertebrates were the most sensitive group (0.36; 0.22 to 0.52), followed by algae (0.45; 0.36 to 0.62), whereas fish were less sensitive (0.46; 0.28 to 0.67). For mixed-target pesticides, algae had the greatest median sensitivity (0.35; 0.16 to 0.50), followed by fish (0.40; 0.29 to 0.54) and invertebrates (0.47; 0.31 to 0.68).

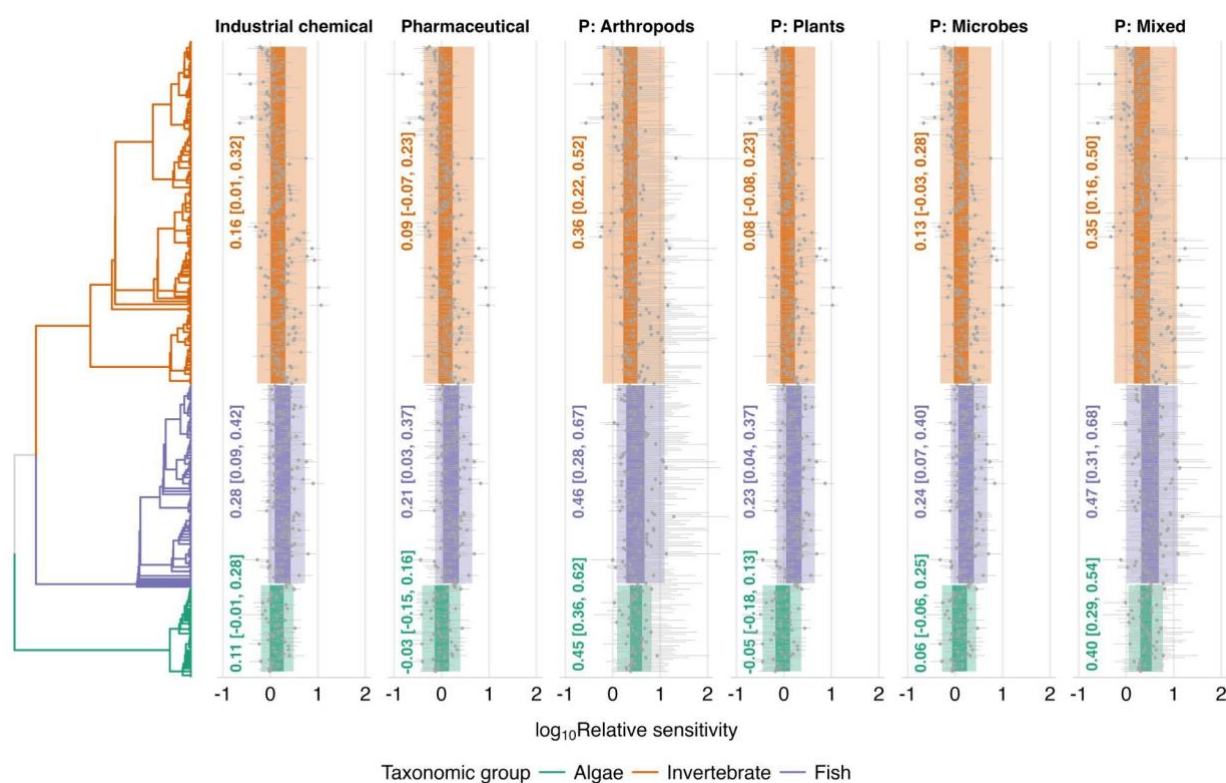


Figure 2. Phylogeny-aligned patterns of relative sensitivity across taxa and chemical-use groups. Left: Genus-level phylogenetic tree, with branch colours indicating the three broad taxonomic groups: algae, invertebrates, and fish. Right: Genus-level relative sensitivity distributions within each chemical-use group: industrial chemical, pharmaceutical, pesticides (P) targeting arthropods, plants, microbes, and mixed targets. Genera are shown in the same vertical order as in the phylogeny. Thin grey horizontal segments show the interquartile range (IQR, 25th–75th percentiles) of $\log_{10}$ relative sensitivity across chemical identities within each chemical-use group, and grey points indicate genus-level medians. Relative sensitivity was calculated as the species LC_{50} normalised to that of *Daphnia magna* for the same chemical identity; values of 0 indicate equal sensitivity to *D. magna*, values < 0 indicate greater sensitivity, and values > 0 indicate lower sensitivity. Within each taxonomic group, shaded bands summarise the distribution of genus-level medians: darker shading indicates the interquartile range (IQR, 25th–75th percentiles) and lighter shading indicates the central 95% range (2.5th–97.5th percentiles).

3.2 Phylogenetic signal in species relative sensitivity

Phylogenetic signals in relative sensitivity, quantified using Pagel's λ and estimated separately for each chemical and taxonomic group, varied substantially from 0.00 to 0.79 (**Figure 3**). A two-way ANOVA showed strong differences among taxonomic groups ($F = 1953$, $df = 2$, $P < 0.001$), weaker but significant differences among chemical-use groups ($F = 11$, $df = 5$, $P < 0.001$), and a significant interaction between taxonomic group and chemical-use group ($F = 18$, $df = 10$, $P < 0.001$).

Differences among taxonomic groups were especially pronounced. Invertebrates showed strong phylogenetic signals, with a median λ of 0.44 (IQR: 0.35 to 0.49). In contrast, both algae and fish showed weak signals, with median λ values close to zero. After Benjamini-Hochberg correction within each taxonomic and chemical-use group combination, the significant phylogenetic signal was detected for 1091 of 1103 chemicals for invertebrates, whereas no chemical-specific tests remained significant for algae or fish. Estimates of phylogenetic signal were robust to progressive exclusion of predicted sensitivity data, with little change in median Pagel's λ after excluding up to 15% of the predicted data (**Figure S4**).

Variation in phylogenetic signals among chemical-use groups was taxon dependent (**Figure 3**). In algae and fish, pesticides targeting arthropods and mixed-target pesticides had significantly higher λ values than other chemical-use groups, although median λ values remained low (**Table S4**). In invertebrates, median λ was highest for industrial chemicals and pharmaceuticals and lowest for mixed-target pesticides, ranging from 0.39 to 0.47 across chemical-use groups.

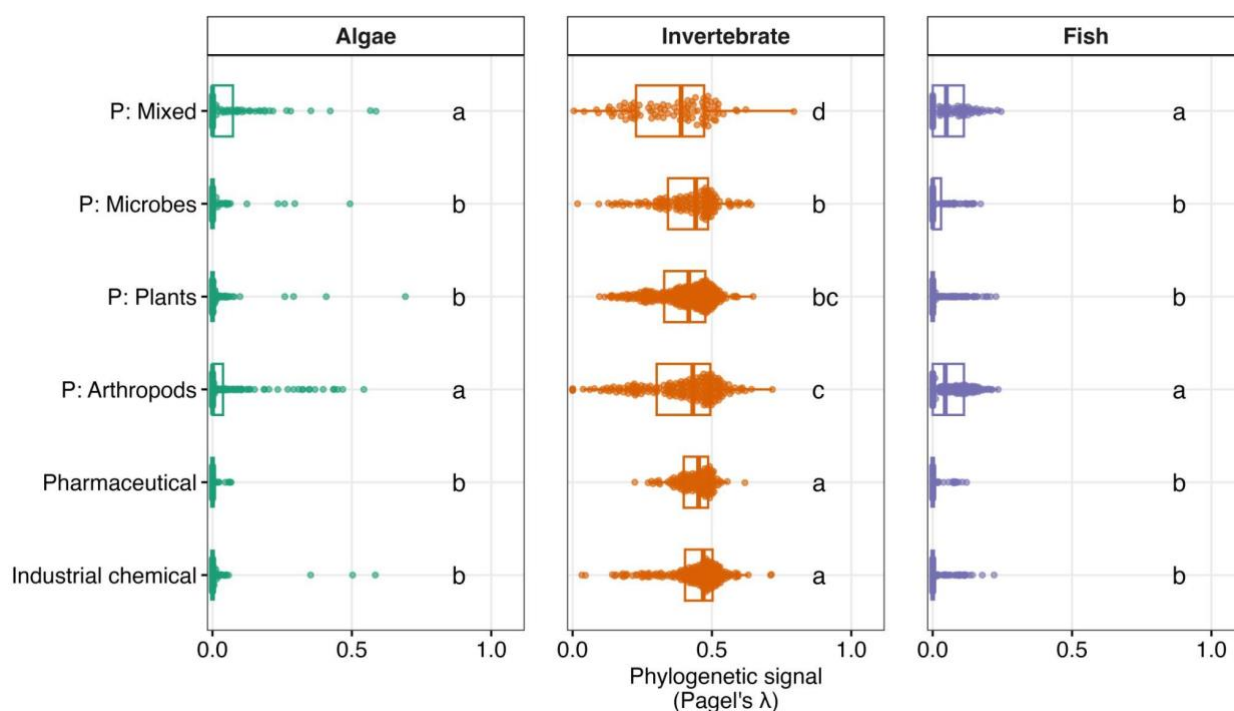


Figure 3. Distribution of phylogenetic signal (Pagel's λ) in species relative sensitivity across chemical-use groups and taxonomic groups. Each point represents one chemical-specific estimate of Pagel's λ based on genus-level mean relative sensitivity, and boxplots summarise the distribution across all chemical identities within each chemical-use group. Boxes show the interquartile range, central lines indicate medians, and whiskers extend to $1.5 \times \text{IQR}$. P denotes pesticides. Lowercase letters indicate significant differences among chemical-use groups within each taxonomic group based on estimated marginal means with Benjamini–Hochberg correction. Groups sharing a letter are not significantly different; within each panel, letter a denotes the group with the highest median Pagel's λ .

3.3 Model support for alternative allometric hypotheses

For each taxonomic and chemical-use group combination, we compared four candidate models (**Table 1**) using LOO cross-validation. Across all 18 taxonomic and chemical-use group combinations, the M3 model had the highest expected log predictive density (ELPD), indicating the strongest predictive performance (**Figure 4**). Model comparison therefore consistently supported the group-specific allometry hypothesis, in which both baseline sensitivity and allometric slopes vary among functional groups.

Differences in ELPD among candidate models were especially pronounced in algae, where the alternative models showed large declines relative to M3 (**Figure 4**). Although the differences were smaller in invertebrates and fish, the same model ranking was retained across all chemical-use groups.

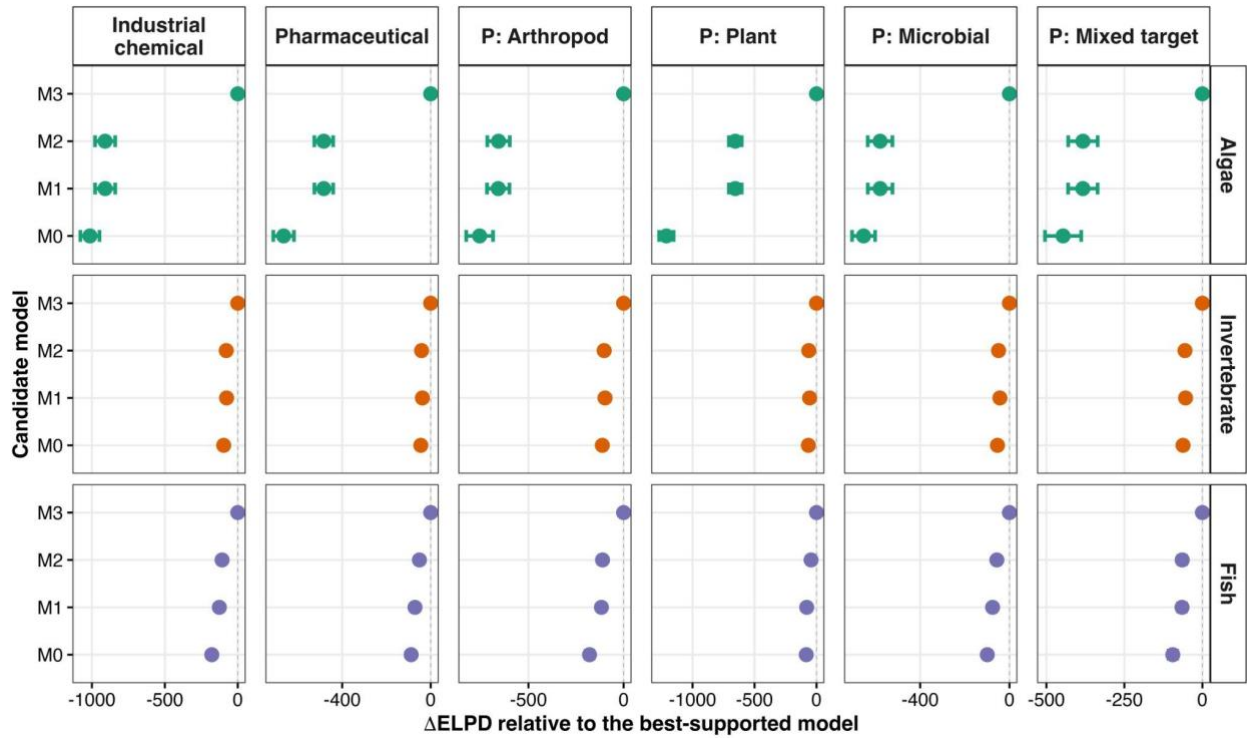


Figure 4. Leave-one-out model comparison across taxonomic and chemical-use groups. Approximate leave-one-out cross-validation was used to compare four candidate Bayesian phylogenetic hierarchical models within each taxonomic group and chemical-use group combination. Points show differences in expected log predictive density (ΔELPD) relative to the best-supported model within each panel, with error bars showing one standard error. Values closer to zero indicate stronger predictive support. Models M0–M3 correspond to the four hypotheses (**Table 1**): H0, null model; H1, global allometry; H2, functional group differences in baseline sensitivity with a shared allometric slope; and H3, functional group-specific allometry, where both baseline sensitivity and allometric slopes vary among functional groups.

3.4 Functional group-specific allometry

Following the consistent support for the functional group-specific allometry model, we assessed whether this model's predictive improvement reflected ecologically meaningful differences in allometric relationships. We estimated posterior effect sizes for functional group-specific slopes and examined pairwise contrasts among functional group-specific slopes and baselines.

Overall, standardised allometric effects were generally weak or uncertain (**Figure 5, Figure S5**). Of the 102 functional group-specific slopes estimated across taxonomic and chemical-use groups, 40 (39%) had 95% HDIs entirely within ± 0.20 ROPE, including 17 (17%) within ± 0.10 . Only 22 (22%) slopes were entirely outside ± 0.20 indicating moderate or stronger allometric effects, while the remaining 40 slopes crossed the ROPE boundary, indicating posterior uncertainty in whether these allometric relationships were ecologically negligible or biologically meaningful. Standardised allometric coefficients were robust to progressive exclusion of predicted sensitivity

estimates, remaining closely aligned with estimates from the complete dataset across exclusion levels (**Figure S6**).

The slopes with 95% HDI entirely outside the ± 0.20 ROPE were concentrated in algae (13/22) (**Figure 5**). “Other algae” showed positive allometric relationships, with the strongest effect observed for pesticides targeting plants ($\beta_{\text{std}} = 2.40$, 95% HDI: 2.03 to 2.74). In contrast, green algae showed consistently negative slopes across all six chemical-use groups ($\beta_{\text{std}} = -0.57$ to -0.13). Diatoms showed positive slopes for industrial chemicals, pharmaceuticals, and pesticides targeting plants and microbes ($\beta_{\text{std}} = 0.34$ to 0.40). Among invertebrates, moderate allometric effects were observed only for arthropod shredders ($\beta_{\text{std}} = 0.37$ to 0.53). Among fish, omnivores showed positive effects exceeding the ROPE for industrial chemicals and mixed-target pesticides ($\beta_{\text{std}} = 0.25$ and 0.26 , respectively), while detritivores/herbivores also exceeded the ROPE for mixed-target pesticides ($\beta_{\text{std}} = 0.58$, 95% HDI: 0.20 to 0.97).

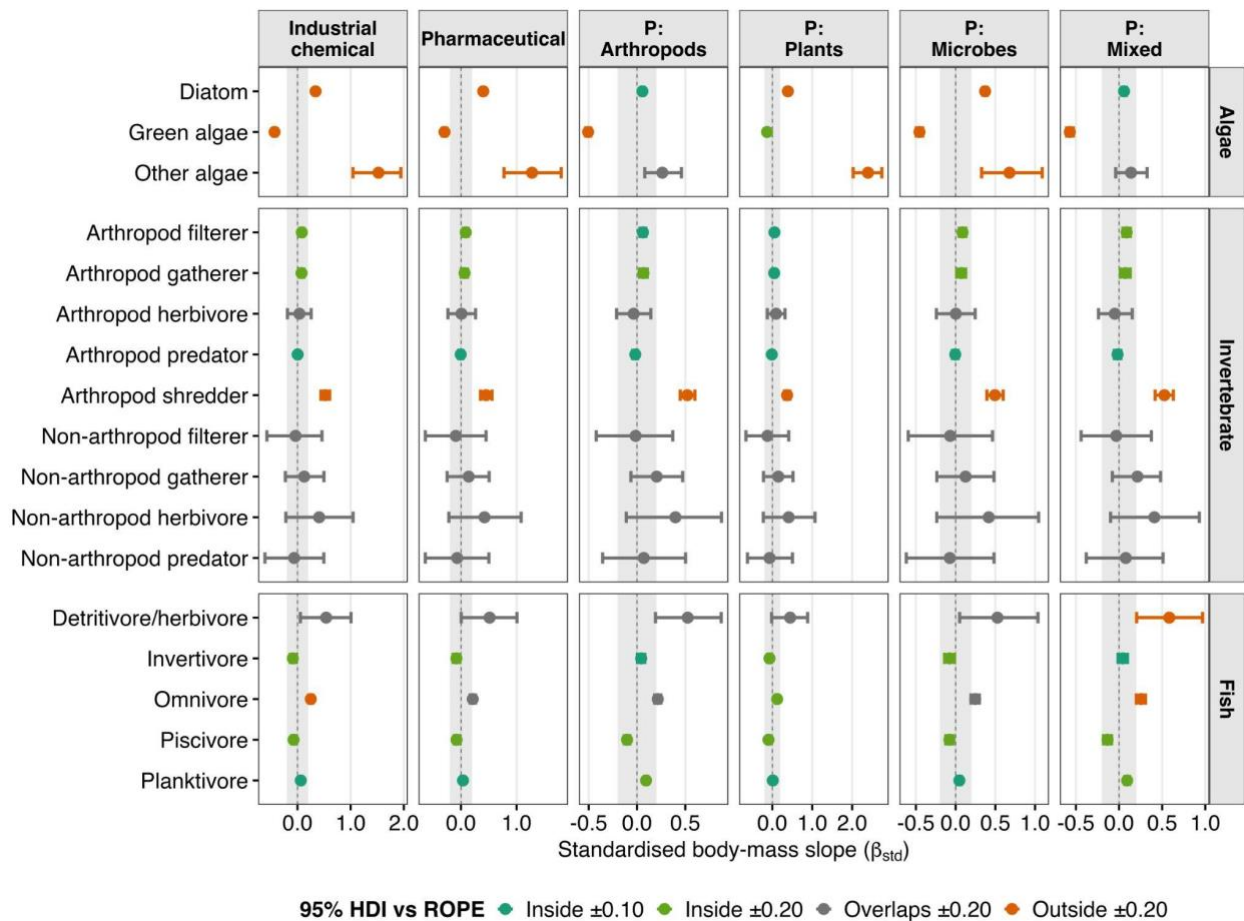
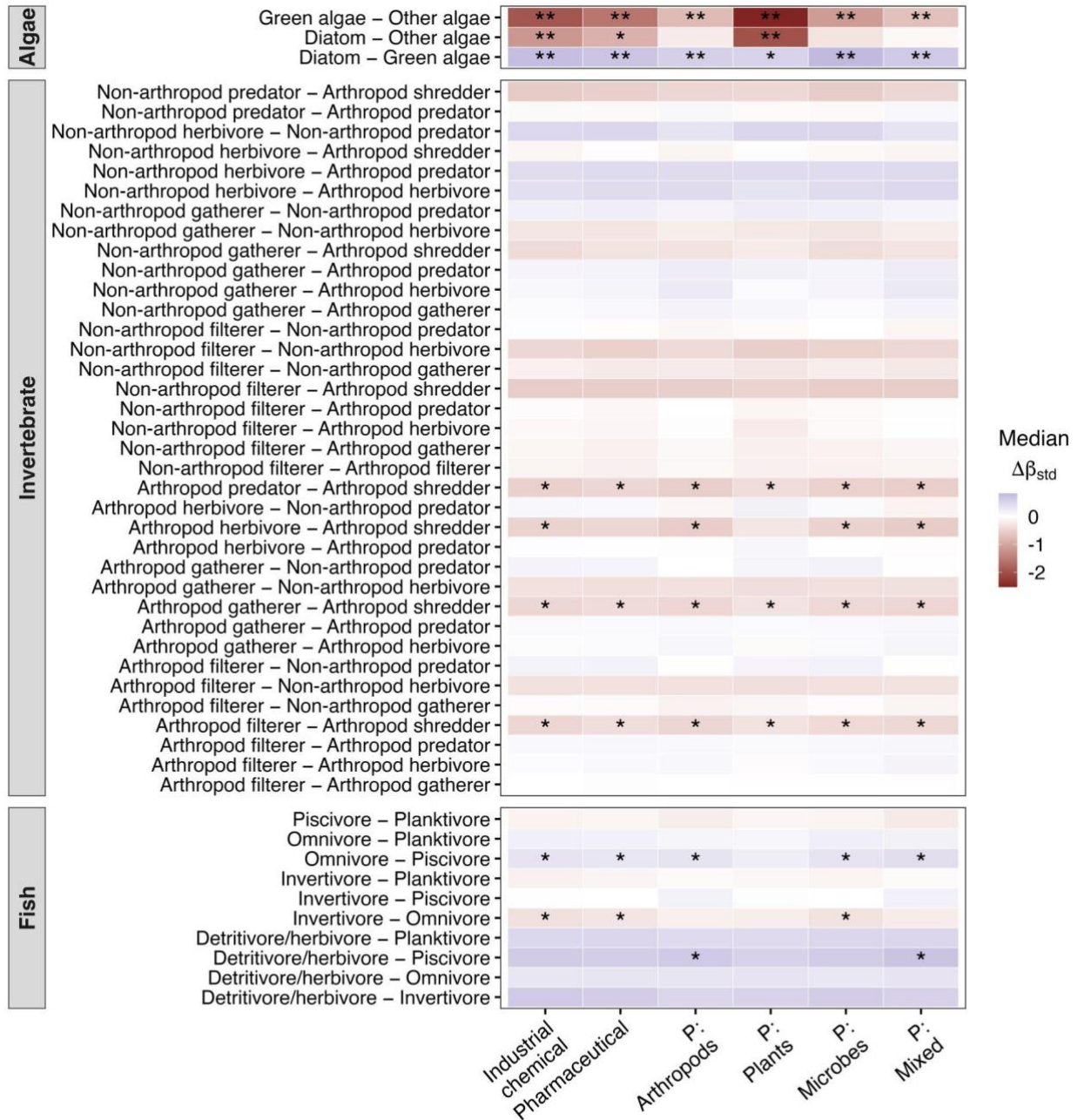


Figure 5. Standardised specific allometric slopes of functional groups across taxonomic groups and chemical-use groups. Posterior estimates of standardised allometric slopes (β_{std}) are shown for each functional feeding group under the best-supported functional group-specific allometry model. Points show posterior medians, and horizontal bars show 95% highest density intervals (HDI). Shaded regions indicate the region of practical equivalence (ROPE) at ± 0.20 . Colours indicate whether the 95% HDI falls entirely within, overlaps, or falls entirely outside the ROPE thresholds.

Pairwise slope contrasts, representing differences in the strength and direction of body mass-sensitivity relationships among functional groups, showed that differentiation in allometric scaling was strongest in algae and more limited in invertebrates and fish (**Figure 6; Figure S7-S9**). Of the 294 pairwise contrasts, 47 (16%) had 95% HDIs entirely outside ± 0.20 , including 13 (4%) outside ± 0.50 . Among the 18 pairwise slope contrasts in algae, 15 had 95% HDIs entirely outside ± 0.20 , including 13 that were also entirely outside ± 0.50 . In invertebrates, 22 of 216 contrasts were outside ± 0.20 , all involving arthropod shredders, which had more positive slopes than other functional groups. In fish, 10 of 60 contrasts were outside ± 0.20 . Omnivores had more positive slopes than piscivores in five chemical-use groups and invertivores in three, while detritivores/herbivores had more positive slopes than piscivores for arthropod-targeting and mixed-target pesticides. Thus, clear slope differentiation was widespread among algal functional groups but concentrated in a small subset of comparisons in invertebrates and fish.



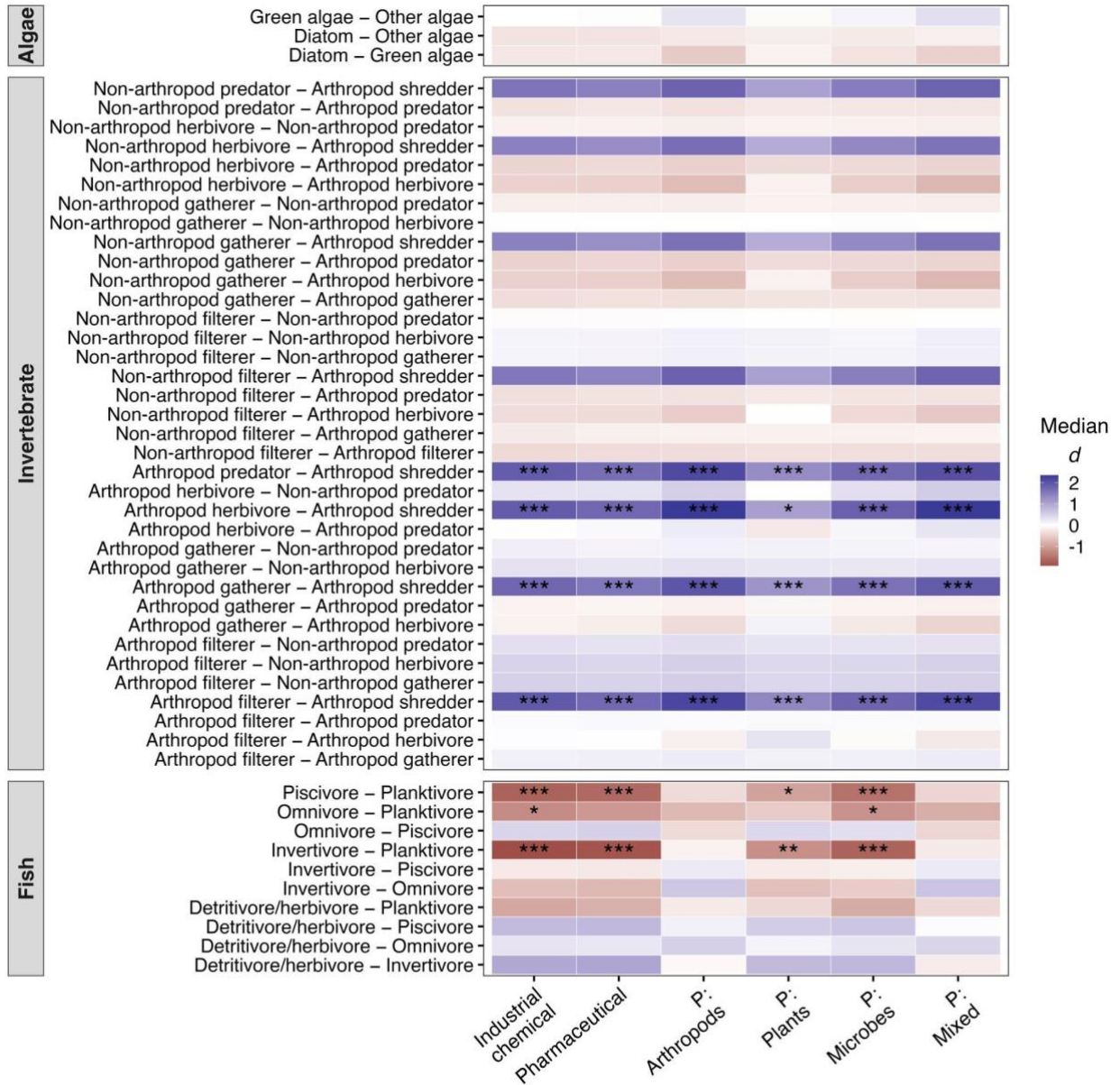
* 95% HDI entirely outside ± 0.20 ; ** 95% HDI entirely outside ± 0.50

Figure 6. Heatmap showing posterior median pairwise contrasts in standardised allometric slopes ($\Delta\beta_{std}$) among functional groups under the best-supported group-specific allometry model. Tile colours show the posterior median slope contrast. Asterisks indicate contrasts whose 95% highest density intervals (HDIs) fall entirely outside regions of practical equivalence (ROPE): * outside ± 0.20 and ** outside ± 0.50 .

Pairwise baseline contrasts showed even less differentiation among functional groups than pairwise slope contrasts (**Figure 7; Figure S7-S9**). Of the 294 baseline contrasts, 34 (12%) had 95% HDIs entirely outside ± 0.20 , including 30 (10%) outside ± 0.50 and 29 (10%) outside ± 0.80 . These contrasts were concentrated in invertebrates and fish, whereas no algal baseline contrast

exceeded the ± 0.20 ROPE. All 24 supported invertebrate contrasts involved arthropod shredders, whose baselines were lower than those of arthropod filterers, gatherers, herbivores, and predators across all six chemical-use groups. All 10 supported fish contrasts involved planktivores, whose baselines were higher than those of invertivores and piscivores for industrial chemicals, pharmaceuticals, and pesticides targeting plants and microbes, and higher than those of omnivores for industrial chemicals and microbe-targeting pesticides. However, most remaining baseline contrasts overlapped the ROPE boundary, indicating uncertainty rather than evidence of negligible differences.

Together, these results indicate that support for functional group-specific allometry was accompanied by uneven differentiation among functional groups. Slope differences were widespread in algae, whereas both slope and baseline differences in invertebrates centred on arthropod shredders. In fish, slope differences mainly involved omnivores, while baseline differences consistently involved planktivores.



* 95% HDI entirely outside ± 0.20 ; ** 95% HDI entirely outside ± 0.50 ; *** 95% HDI entirely outside ± 0.80

Figure 7. Pairwise contrasts in baseline sensitivity among functional groups under the best-supported group-specific allometry model. Baseline contrasts compare functional group-specific intercepts at the corresponding dataset's mean $\log_{10}$ body mass. For each posterior draw, standardised contrasts were calculated as $d = \frac{\alpha_i - \alpha_j}{\sigma}$, where α_i and α_j are the functional group-specific intercepts for two functional groups, and σ is the residual standard deviation. Tile colours show posterior median d for the first functional group listed minus the second. Asterisks indicate contrasts whose 95% highest density intervals (HDIs) fall entirely outside regions of practical equivalence (ROPE): * outside ± 0.20 and ** outside ± 0.50 , and *** outside ± 0.80 .

3.5 Explained variation and random-effect variance partitioning

Although functional group-specific allometry consistently improved predictive performance, the fixed effects, functional group identity and functional group-specific body-mass scaling, explained

only a modest proportion of variation in relative sensitivity (**Figure 8a**). Marginal Bayesian R^2 , representing fixed-effect variance relative to the combined fixed-effect, random-effect, and residual variance, ranged from 0.03 to 0.37 across taxonomic group and chemical-use group combinations (**Figure 8a**). Fixed effects explained the largest share of variation in algae, with marginal R^2 values of 0.17–0.37, but contributed little in invertebrates (0.05–0.06) and fish (0.03–0.05).

In contrast, conditional R^2 , which includes variance associated with both fixed and random effects relative to total variance, was substantially higher, ranging from 0.77 to 0.93. Mean conditional R^2 remained high across algae, invertebrates, and fish, at 0.85, 0.80, and 0.90, respectively. Correspondingly, the residual proportion of total variance, calculated as $1 - \text{conditional } R^2$, accounted for 7–23% of total variance. On average, residual variance represented 15% of total variance in algae, 20% in invertebrates, and 10% in fish. The large difference between marginal and conditional R^2 indicated that much of the explained variation was associated with chemical identity and phylogenetic structure rather than the fixed effects.

Random-effect variance was dominated by phylogenetic structure rather than chemical identity in most combinations (**Figure 8b**). Across all models, phylogenetic variance accounted for 59–97% of total random-effect variance, whereas chemical identity accounted for 3–41%. The phylogenetic contribution was greatest in invertebrates, ranging from 92% to 97% and averaging 95% across chemical-use groups, consistent with their high Pagel's λ (**Figure 3**). In fish, phylogenetic structure accounted for 77–91% of random-effect variance. Algae showed the greatest variation in the relative contributions of the two random effects, with chemical identity accounting for approximately 41% of random-effect variance for both arthropod-targeting and mixed-target pesticides, compared with 4–19% for the remaining chemical-use groups.

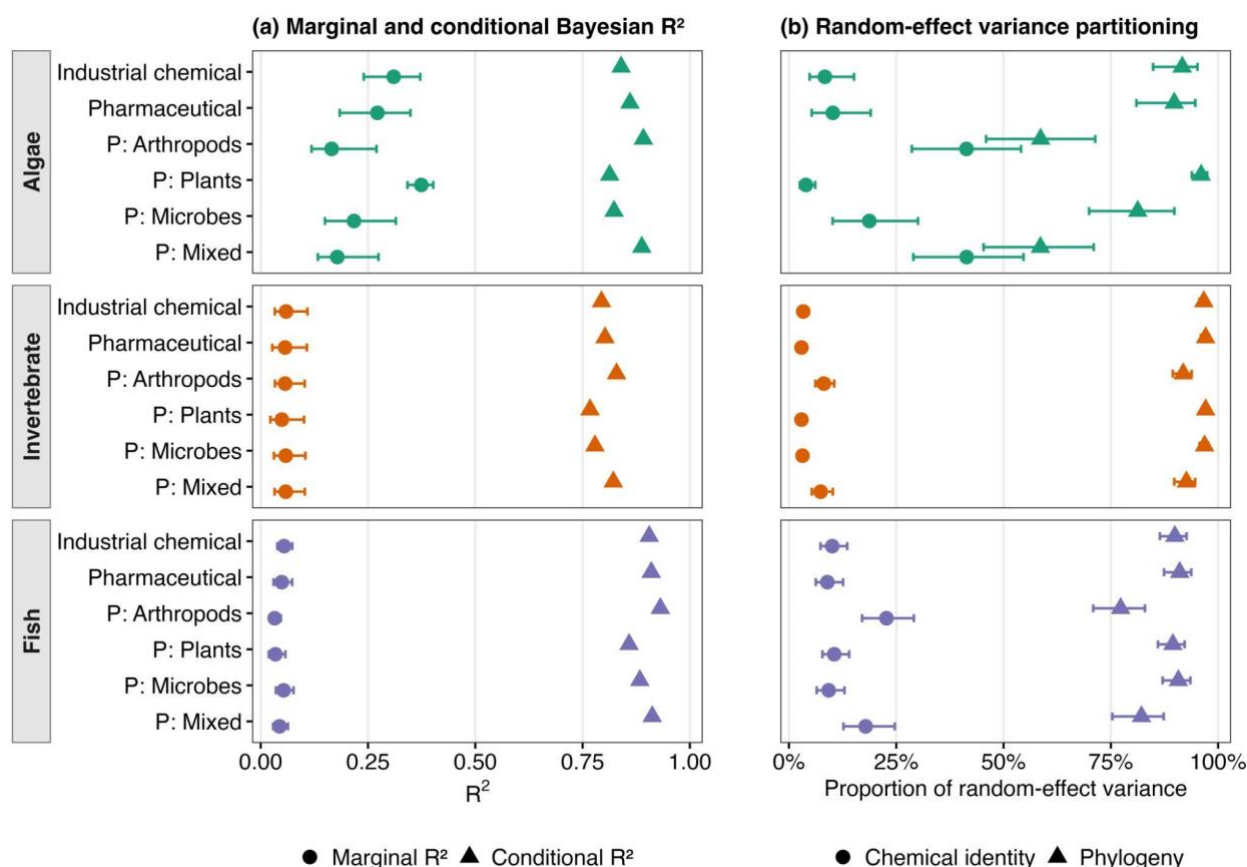


Figure 8. Model explanatory power and random-effect variance partitioning across taxonomic groups and chemical-use groups. (a) Marginal and conditional Bayesian R^2 for the best-supported group-specific allometry model for each taxonomic group and chemical-use group combination. Marginal R^2 represents the fixed-effect variance relative to total variance, whereas conditional R^2 represents the combined fixed-effect and random-effect variance relative to total variance. Points show posterior estimates, and horizontal bars show 95% credible intervals. (b) Partitioning of random-effect variance between chemical identity and phylogenetic structure.

4. Discussion

A fundamental challenge for higher-tier chemical risk assessment is how to incorporate a diversity of species and their variation in chemical sensitivity into predictive, risk assessment frameworks. This is particularly difficult when direct measurements of sensitivity are too sparse to enable risk assessment at higher levels of biological organisation. In ecology, part of this challenge has been addressed through body-size scaling, because key biological traits such as metabolism, production and foraging often scale predictably with body mass that underpin biodiversity dynamics. If chemical sensitivity also exhibited a general allometric structure, body mass could provide a practical link between species-level sensitivity information and process-based food web community models. Identifying general principles that link variation in chemical sensitivity to the trait-based structure of ecological communities may therefore provide an important bridge for

higher tier chemical risk assessment. In this study, we assembled an extensive dataset integrating species sensitivity, functional group, phylogenetic relatedness and the ecological master trait of body mass to evaluate whether body mass provides a general allometric basis for predicting species relative sensitivity across aquatic taxa and chemical-use groups.

Overall, we found that body mass was a weak predictor of sensitivity across the aquatic taxa and chemical-use groups examined, suggesting limited generality of the allometric relationships reported in studies with narrower taxonomic and chemical coverage. Although models allowing allometric relationships to vary among functional groups consistently showed the best predictive performance, most allometric slopes were weak, with moderate effects restricted to a few functional groups. Phylogenetic relatedness and chemical identity captured substantial additional variation beyond the measured traits. Phylogeny accounted for the largest share of random-effect variance in most models, even though phylogenetic signal in relative sensitivity was strong in invertebrates but weak in algae and fish. In the following sections, we examine the strength and context dependence of allometric relationships, the role of phylogenetic structure in cross-species extrapolation, variation in sensitivity patterns among chemical-use groups, and the implications for food web-level risk assessment.

4.1 Functional group-specific allometry improves predictive performance, but allometric effects are generally weak

Across all combinations of taxonomic group and chemical-use group, model M3 had the highest predictive performance, indicating that allowing body mass-sensitivity relationships to vary among functional groups provided useful predictive information. However, the magnitude of these relationships differed among taxa. Several algal functional groups showed moderate to strong allometric effects and pronounced differences in slopes. In contrast, slopes were generally weaker in invertebrates and fish, although some functional groups differed substantially in baseline sensitivity. Thus, the improved predictive performance of M3 did not indicate consistently strong allometric scaling. Functional groups primarily distinguished allometric relationships in algae, but mostly captured differences in average sensitivity among invertebrates and fish.

One possible explanation for the stronger allometric patterns in algae is that body mass is more directly linked to chemical uptake and sensitivity. In unicellular algae, body mass largely reflects cell size, which determines the surface area available for chemical exchange relative to cell volume and is also associated with growth and metabolic rates. Cell size has consequently been linked to chemical uptake and sensitivity, although these relationships vary among chemicals and species⁵⁹. In multicellular animals, whole-body mass is a less direct measure because chemical

uptake and processing also depend on ventilation, lipid content, metabolism, and life stage⁶⁰, which may weaken general body mass-sensitivity relationships in invertebrates and fish.

Previous studies have reported strong allometric relationships between body mass or length and chemical sensitivity^{21,24,25,30,61}. Such relationships may be important within particular taxonomic groups or for particular chemicals. However, when phylogeny is not considered, estimated body-size effects may also include variation associated with shared evolutionary history because body mass is itself phylogenetically structured³⁴. Our results are therefore consistent with the possibility that some variation attributed to body size is instead associated with phylogenetic relatedness. A similar pattern has been reported for fish: body length and life-history and ecological traits such as migration type and air-breathing ability, were associated with LC₅₀ values for 269 fish species and 29 chemicals, but these associations were only detected when phylogeny was not accounted for³⁷. However, this does not mean that body size is never important. For example, Pamminer found strong relationships between bee body weight and sensitivity to insecticides, and such relationships occur independently of phylogeny²³.

Uncertainty in the sensitivity estimates and trait data may also have influenced the estimated allometric relationships. Sensitivity values were predicted rather than directly observed, and species-level body mass and functional group classifications may not represent the life stages used in the underlying toxicity tests. For fish, for example, traits describing adults may be poorly matched to tests conducted on juveniles or early life stages. Ontogenetic changes in body size and feeding ecology could therefore affect the estimated trait-sensitivity relationships. We did not quantify these effects, so their contribution to the weak allometric patterns remains uncertain.

4.2 Invertebrate relative sensitivity is strongly structured by phylogeny

Compared with algae and fish, we found invertebrates showed stronger phylogenetic signals in relative sensitivity. Pagel's λ estimates, marginal and conditional R^2 , and random-effect variance partitioning consistently identified shared phylogenetic relatedness as a major source of variation in invertebrate sensitivity. Differences among candidate models (M0-M3) were also relatively small, partly because the baseline model, which included a phylogenetic random effect, already captured a large proportion of the structured variation. By contrast, body mass and functional group-specific allometry added little explanatory information, with a clear allometric effect detected for only one invertebrate functional group.

We further found that the strong invertebrate-wide pattern was partly driven by differences among major invertebrate taxonomic groups (**Appendix S2, Figure S10**). Finer-scale phylogenetic structure was also evident within some clades, most clearly in crustaceans, whereas estimates for insects, annelids, and molluscs were weaker and more variable (**Appendix S2, Figure S11**). These

differences may reflect weaker phylogenetic structuring within some groups, although differences in taxonomic coverage and sample size may also affect the estimates and their precision. Together, these analyses suggest that the invertebrate-wide pattern reflects both broad differences among major groups and phylogenetic structure within some clades.

Previous studies likewise indicate that taxonomic and phylogenetic relatedness can strongly structure chemical sensitivity. Taxonomic patterns have been demonstrated for species responses to insecticides⁶², herbicides⁶³, and fungicides⁶⁴. More explicitly phylogenetic analyses have also reported strong signal in macroinvertebrate pollution responses at the genus level⁶⁵ and linked dissolved cadmium susceptibility in aquatic insects to phylogenetically structured ecophysiological differences⁶⁶. Strong phylogenetic signal has also been reported for algae⁶⁷ and fish³⁸ under particular chemical and taxonomic contexts. Across our broader dataset, phylogenetic structure was strongest and most consistent in invertebrates. Nevertheless, phylogeny remained the dominant source of random-effect variance in algae and fish after accounting for body mass and functional group, despite their generally weaker Pagel's λ estimates. The taxonomic groups therefore differed in the strength of phylogenetic structuring rather than in its complete presence or absence.

The strong phylogenetic structure in invertebrate relative sensitivity has important implications for cross-species extrapolation in ecological risk assessment. When empirical toxicity data are sparse, phylogenetic information can provide a biologically informed basis for predicting the sensitivity of untested invertebrate species. Recent developments in hierarchical species sensitivity distribution (hSSD) models have enabled sensitivity prediction for untested invertebrate species using taxonomic relatedness^{43,44}. Our results suggest that explicit phylogenetic information could provide an alternative or complementary structure for such extrapolations. Phylogeny-based prediction is already widely used to estimate missing species functional traits, particularly when traits show strong phylogenetic structure⁶⁸. For example, tools such as PhyloPars use evolutionary relatedness among species to infer missing trait values⁶⁹. We applied this tool to species relative sensitivity by randomly masking genus-chemical sensitivity values and predicting them from phylogenetic relatedness using PhyloPars. This cross-validation analysis showed high predictive accuracy for invertebrate relative sensitivity, with strong correlations between PhyloPars predictions and machine learning predicted values across masking levels (**Figures S12-S13**; Pearson's r generally ≥ 0.95). Correlations with observed sensitivity were also high, although more variable across chemical-use groups ($r = 0.67$ to 0.90). When more species toxicity data were available for model fitting (30% masking), standardised prediction errors were generally concentrated within ± 2 standard errors relative to both machine-learning predicted and observed sensitivity values, except for mixed-target pesticides (**Figure S14**). These results support the potential use of phylogenetic relatedness for predicting sensitivity in poorly tested invertebrate taxa.

Several other phylogeny-informed approaches have also been developed to predict species sensitivity, including models based on phylogeny only⁷⁰ and bilinear models that combine phylogeny with chemical properties⁷¹. The latter explained 77–84% of variability in the acute pesticide toxicity of broad species⁷¹, and 70–80% of variation in macroinvertebrate sensitivity to heavy metals⁷².

4.3 Chemical-use groups modify sensitivity variation, but general biological structure is retained

Chemical-use groups modified the magnitude and ranking of species relative sensitivity, reflecting differences in chemical targets and toxic modes of action that can shift sensitivity distributions towards the taxa or biological processes targeted by each chemical group. However, broad use categories do not fully capture variation among individual chemicals. Chemicals within the same use category can differ in toxic mode of action, uptake pathways, bioavailability, and other chemical-specific properties⁴⁷. Consistent with this, chemical-level random effect in our Bayesian models remained important within chemical-use groups, suggesting that chemicals assigned to the same broad category can still produce varying sensitivity patterns, in part due to differences in toxic mode of action¹².

Despite this chemical-specific variation, the main sources of biological structure in species relative sensitivity were generally consistent within each taxonomic group and across chemical-use groups. Phylogenetic relatedness remained the strongest and most consistent source of biological structure across these groups, particularly in invertebrates. By contrast, functional groups and body mass provided weaker and more context-dependent information. Thus, chemical-use groups modified sensitivity patterns but did not override the broader phylogenetic, functional, and allometric organisation of sensitivity across aquatic taxa.

Phylogenetic signal also varied substantially among individual chemicals within each taxonomic and chemical-use group (**Figure 3, Figure S11**), with some chemicals showing strong signal and others showing little or none. This variation suggests that classification by intended chemical use alone may not fully capture the biological targets or toxicological mechanisms that shape species sensitivity. Future analyses should therefore consider species traits and phylogeny alongside chemical-specific information, such as modes of action and physicochemical properties, to better account for variation among chemicals.

4.4 Implications for food web-level risk assessment

Chemical risk assessment at the food web level requires connecting species-level toxicity information with community-level ecological dynamics. Chemical exposure affects target species

through changes in survival or growth, and these target toxic effects can propagate through trophic interactions and generate non-target toxic effects^{3,9,73}. As a result, food web responses depend not only on network structure, but also on where sensitive species are located within the network. Predicting food web level risk thus requires approaches that assign chemical sensitivity to species in a biologically realistic way^{2,11,74}.

Our findings provide a basis for making these assignments when empirical toxicity data are sparse. Specifically, sensitivity variation follows taxon-specific biological structure: algae showed the clearest signal of allometric structure, invertebrate sensitivity was strongly structured by phylogeny, and fish sensitivity was more closely associated with phylogenetic structure than with allometry. These patterns suggest that sensitivity assignment in food web applications may benefit from some degree of taxon-specific framing rather than relying on a single general predictor. The Bayesian framework also offers a way to represent uncertainty in sensitivity assignments. Joint draws from posterior predictive distributions could generate alternative sets of species sensitivities for repeated food web simulations, preserving the dependencies represented in the model. Combined with uncertainty in the underlying machine-learning predictions, these simulations could assess how uncertainty in sensitivity translates into variation in predicted biomass, species persistence, and community stability. Uncertainty analysis could then identify which species–chemical estimates most influence the predicted outcomes and where additional toxicity measurements would be most informative.

More broadly, this study shows how species traits and evolutionary relationships can inform chemical risk assessment beyond the limited set of organisms tested experimentally. By identifying both structure in chemical sensitivity and the limits of general allometric relationships, our findings provide a basis for cross-species extrapolation that accounts for biological diversity. Building on this foundation, integrating sensitivity estimates and their uncertainty into food web models could extend these insights to the consequences of chemical exposure for biodiversity and ecosystem functioning.

Data and code availability statement

All data and analysis scripts required to reproduce this study are archived in a public Zenodo repository (<https://doi.org/10.5281/zenodo.23559789>).

Author Contributions

Conceptualization: XL, APB. Data curation: XL, AO, RL. Formal analysis: XL. Funding acquisition: APB, LM. Methodology: XL, APB, TFJ, DZC, LM. Investigation: XL, APB. Visualization: XL. Writing – original draft: XL. Writing – review and editing: all authors.

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Supporting Information

Functional group classifications and dataset sample sizes; model diagnostics and posterior predictive checks; comparisons of phylogenetic signal among chemical-use groups; machine-learning prediction validation and sensitivity matrices; robustness analyses excluding predicted estimates; functional group-specific allometric relationships and posterior distributions; phylogenetic analyses within and between major invertebrate lineages; PhyloPars prediction performance and standardised prediction errors (PDF).

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