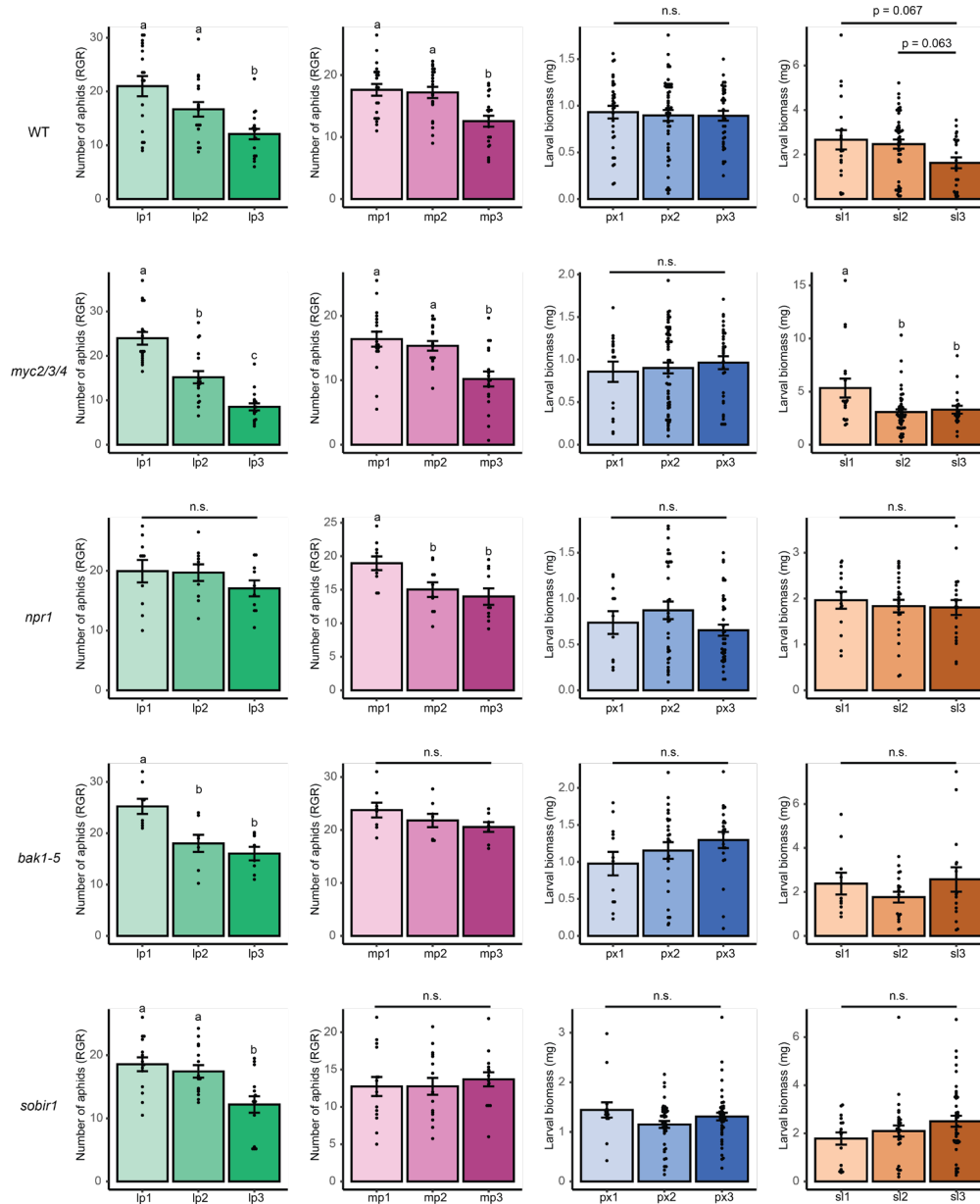
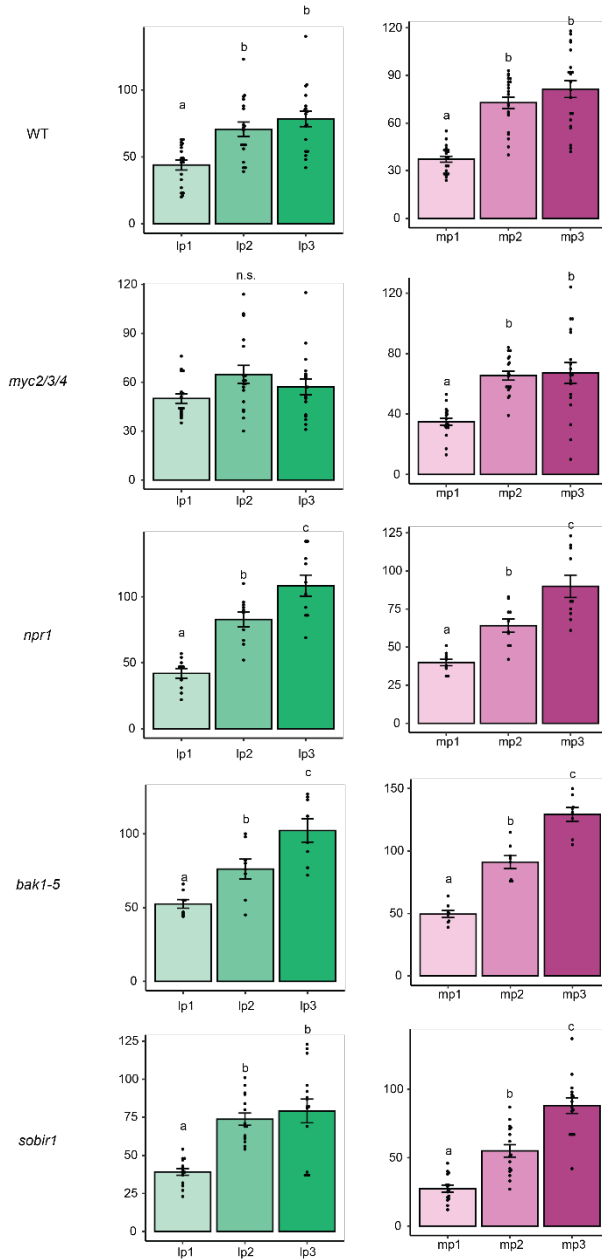


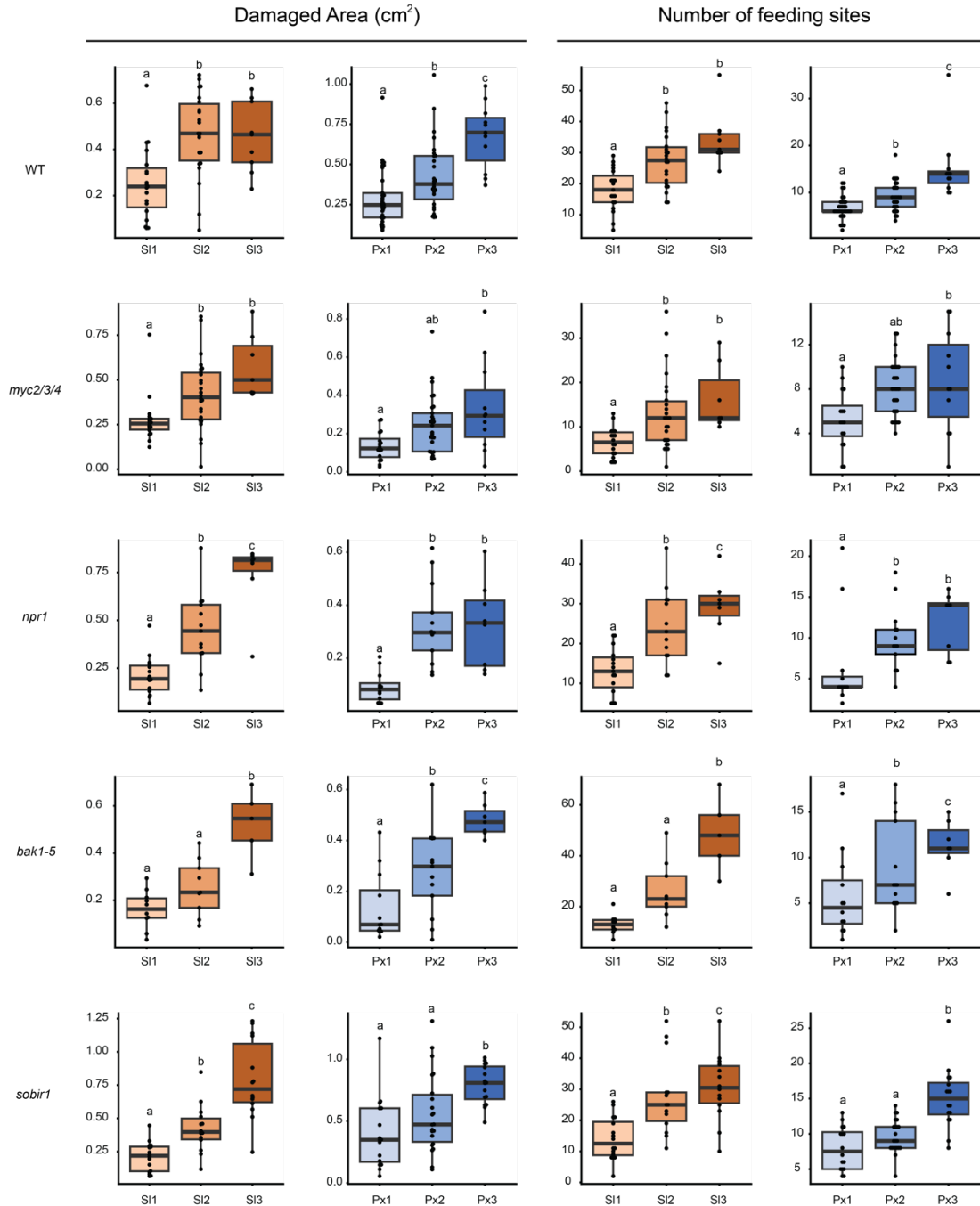
Supplementary Information



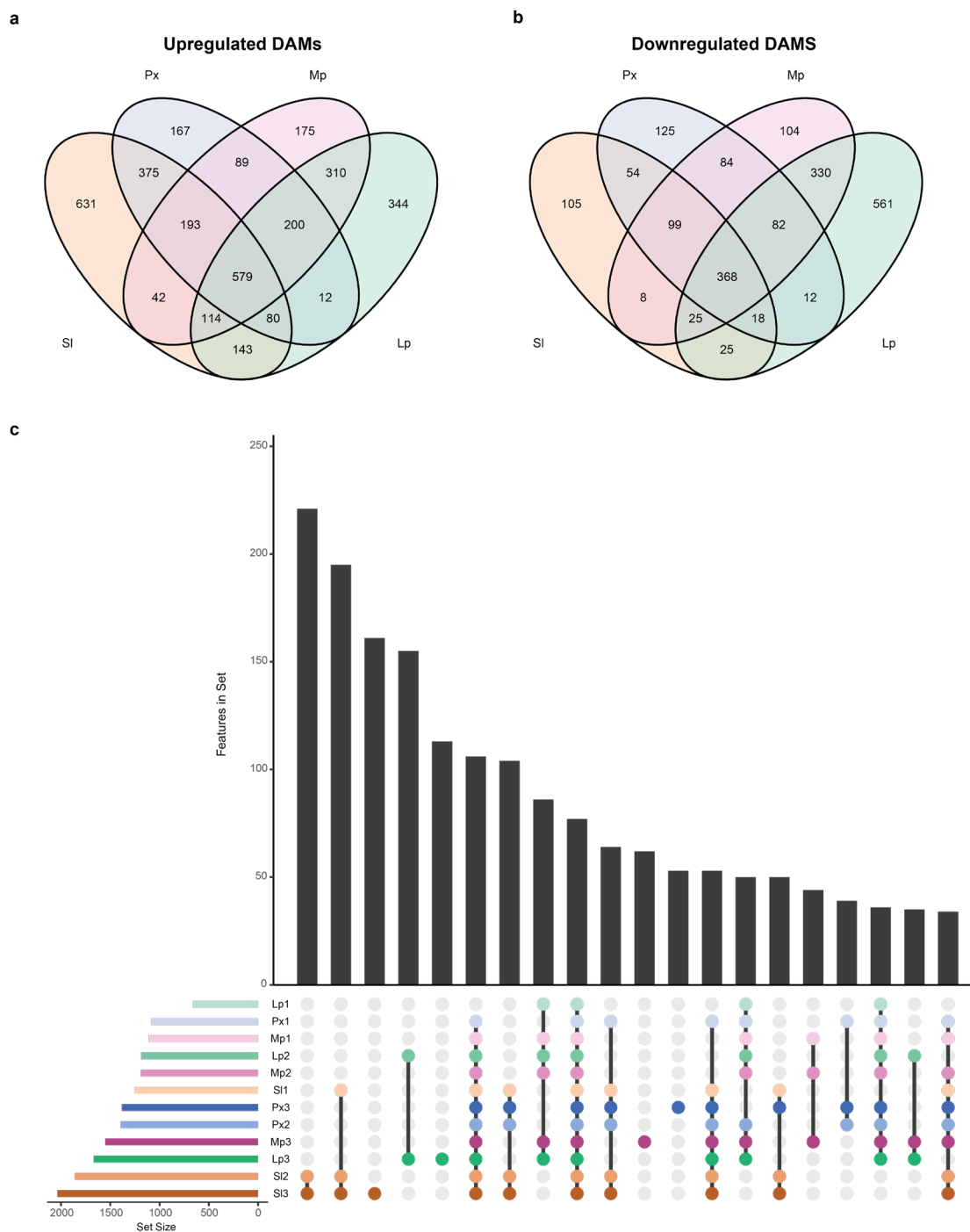
Supplementary Fig. 1. Performances of four herbivores fed on *Arabidopsis thaliana* in different intensities of attack. Numbers of aphids were normalized to relative growth rate by the initial release numbers. Each bar represents mean values with standard errors. Different letters on the bar indicate statistically significant difference (one-way ANOVA followed by Tukey's HSD, $p < 0.05$). The numbers of biological replicates are documented in the Source Data file.



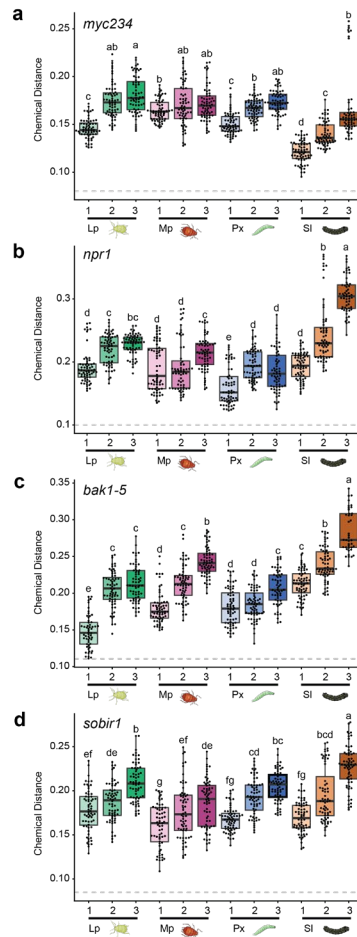
Supplementary Fig. 2. Total number of aphids were counted after 6 days of feeding on. Each bar represents mean values with standard errors. Different letters on the bar indicate statistically significant difference (one-way ANOVA followed by Tukey's HSD, $p < 0.05$). The numbers of biological replicates are documented in the Source Data file.



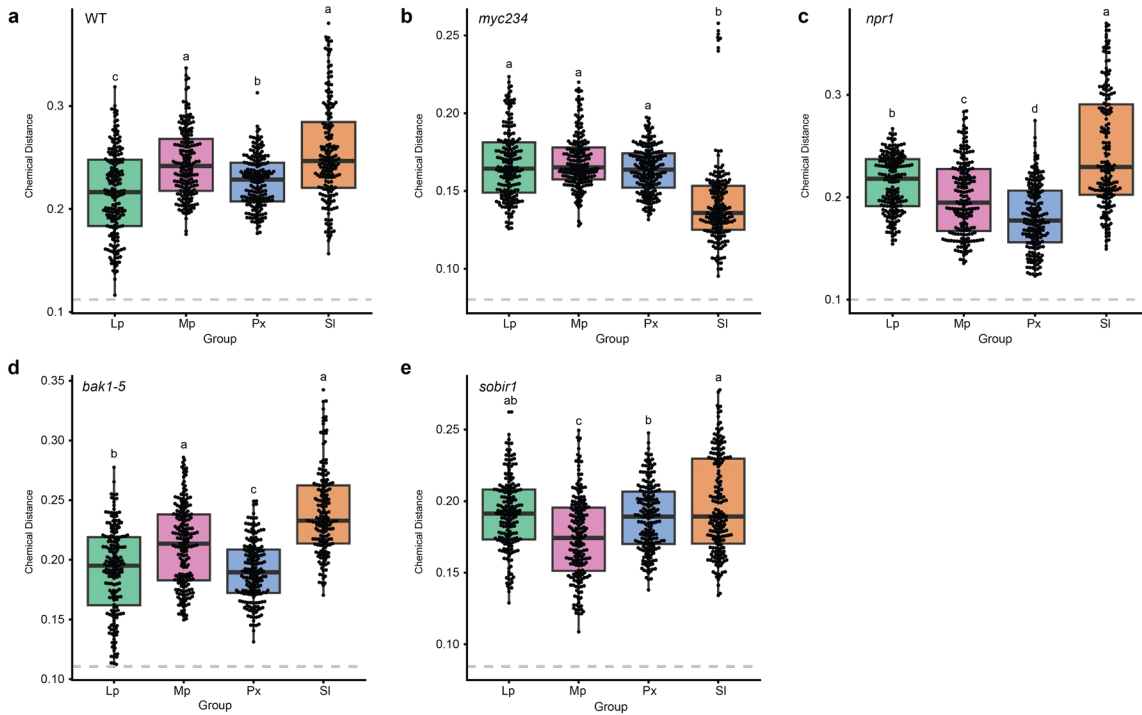
Supplementary Fig. 3. Quantification of damaged area and the number of feeding sites by chewing insects. Each box shows the median as the center line and the 25th and 75th percentiles as the lower and upper bounds. Whiskers extend to the 1.5 IQR. Different letters on the box indicate statistically significant difference (one-way ANOVA followed by Tukey's HSD, $p < 0.05$). The numbers of biological replicates are documented in the Source Data file.



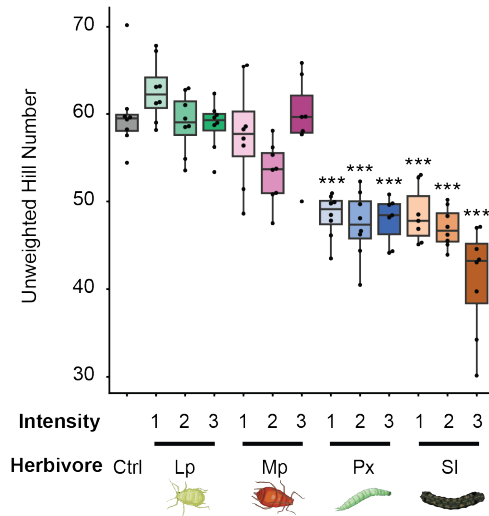
Supplementary Fig. 4. Differentially accumulated molecular features (DAMs) in herbivore-induced metabolomes of WT plants. (a-b) Venn diagram of (a) upregulated and (b) downregulated DAMs identified. (c) UpSet plot of upregulated DAMs with attack intensities separated.



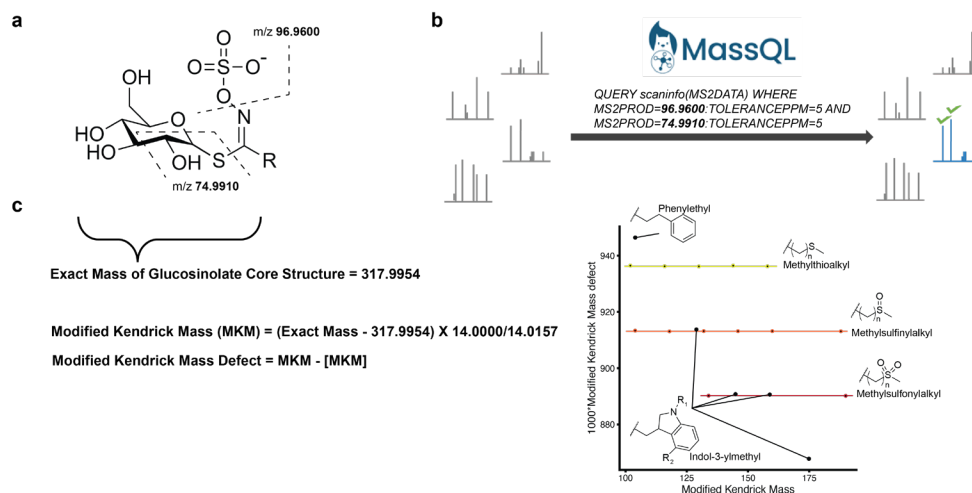
Supplementary Fig. 5. The UniFrac distances between herbivore-induced plants and the control plants, for the following genotypes (a) *myc2/3/4*, (b) *npr1*, (c) *bak1-5*, and (d) *sobir1*. The grey horizontal dashed lines designate mean pairwise distance within the control group. Each box shows the median as the center line and the 25th and 75th percentiles as the lower and upper bounds. Whiskers extend to the 1.5 IQR. Different letters on the boxes indicate statistically significant differences (one-way ANOVA followed by Tukey's HSD, $p < 0.05$)



Supplementary Fig. 6. The UniFrac distances between herbivore-induced plants and the control plants, which of genotypes are (a) WT, (b) *myc2/3/4*, (c) *npr1*, (d) *bak1-5*, and (e) *sobir1*. Groups of same herbivore and different intensities are merged. The grey horizontal dashed lines designate mean pairwise distance within the control group. Each box shows the median as the center line and the 25th and 75th percentiles as the lower and upper bounds. Whiskers extend to the 1.5 IQR. Different letters on the boxes indicate statistically significant differences (one-way ANOVA followed by Tukey's HSD, $p < 0.05$)



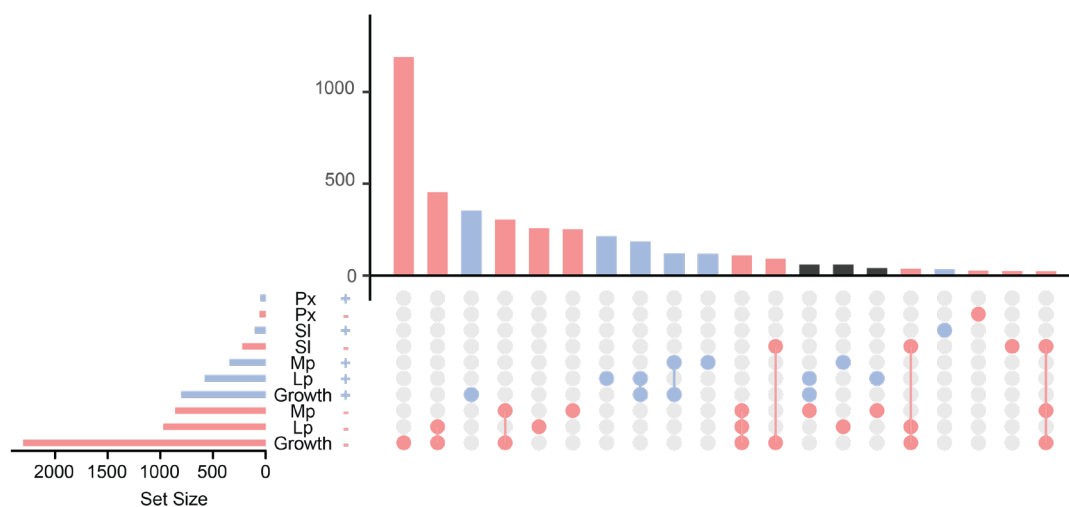
Supplementary Fig. 7. Functional Hill numbers without weights by DreaMS embedding-based distance ($q = 3$) of WT plants induced by herbivores. Each box shows the median as the center line and the 25th and 75th percentiles as the lower and upper bounds. Whiskers extend to the 1.5 IQR. The asterisks indicate significant difference from the control group. (one-way ANOVA followed by Dunnett's test; ***, $p < 0.005$).



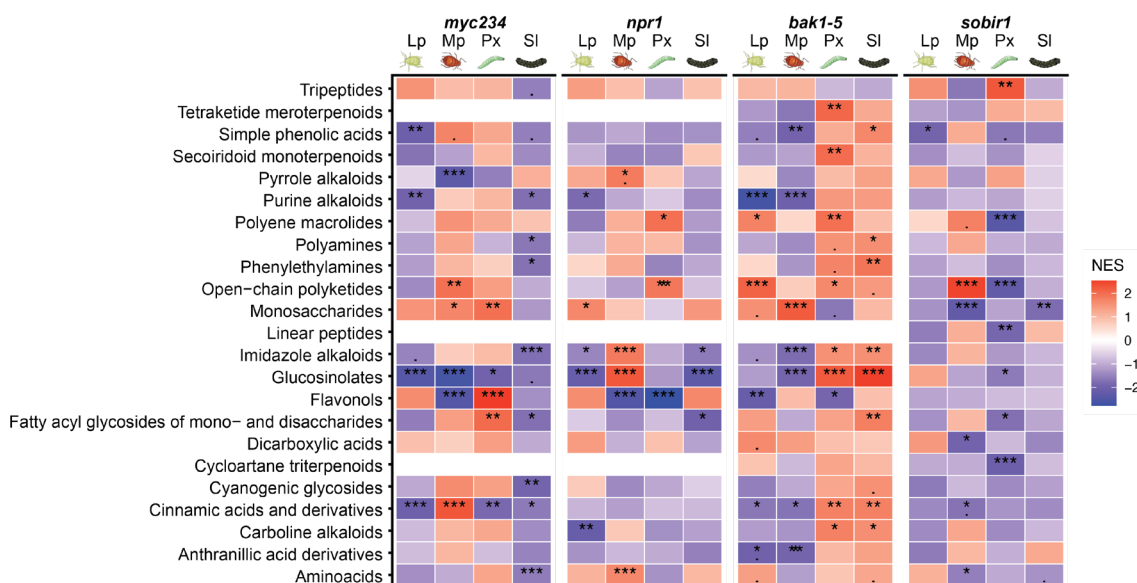
Supplementary Fig. 8. Annotation of glucosinolates. (a) Structure of the core scaffold of glucosinolates and diagnostic fragment ions. (b) MassQL querying diagnostic ions of glucosinolates. (c) Modified Kendrick mass defect of each glucosinolate is plotted with modified Kendrick mass to visualize methionine-derived glucosinolates with different chain lengths along horizontal lines.



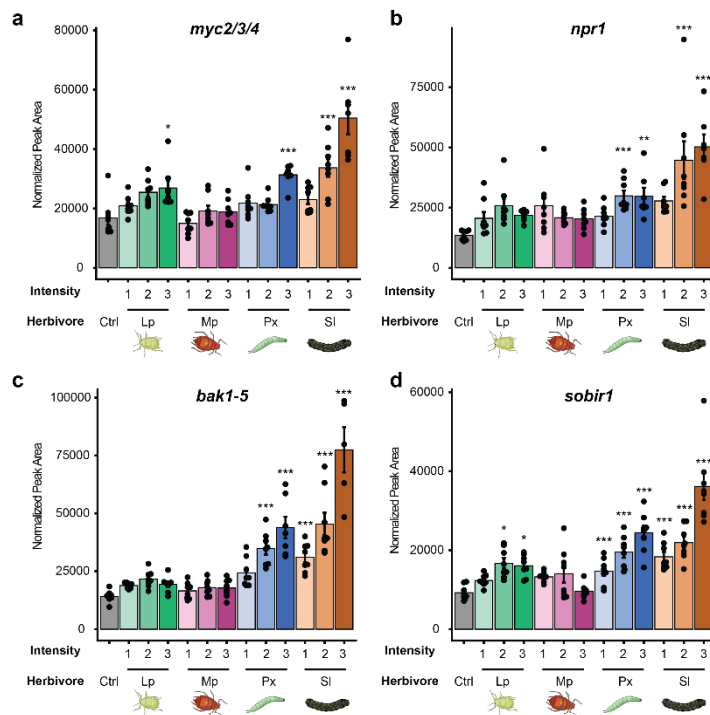
Supplementary Fig. 9. MSEA of node properties (Betweenness, Closeness, Degree Centrality, and Eigenvector centrality) of features in GGM-based co-association network. Only significantly enriched terms are shown. The significance of enrichment was evaluated by MSEA that was performed using a directional (one-sided) permutation-based test.



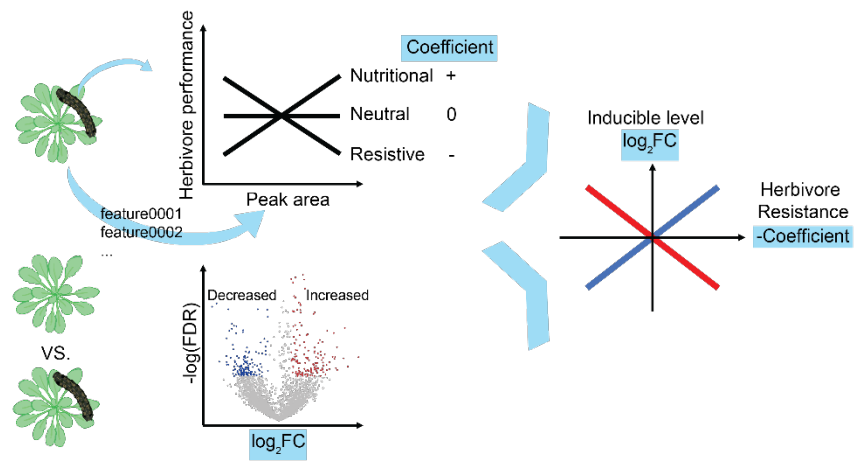
Supplementary Fig. 10. UpSet plot of molecular features correlated with herbivore performances and plant growth. The directionalities of correlations are designated in color.



Supplementary Fig. 11. The normalized enrichment scores (NESs) of MSEA performed on the correlation coefficients of peak area and herbivore performances are visualized by a **heat map**. NC terms that were significantly enriched at least once are used. MSEA was performed using a directional (one-sided) permutation-based test. The asterisks indicate statistical significance of the enrichment (., $p < 0.1$; *, $p < 0.01$; **, $p < 0.001$)



Supplementary Fig. 12. Quantification of normalized peak area of allantoin across all herbivore-treated groups of (a) *myc2/3/4*, (b) *npr1*, (c) *bak1-5*, and (d) *sobir1* plants. The bars represent the mean values with standard errors (*, $p < 0.05$; *, $p < 0.005$; one-way ANOVA followed by Dunnett's test).**



Supplementary Fig. 13. Analytical scheme of the phenotype-based correlation analysis.

Supplementary Table 1.

p values of pairwise PERMANOVA between herbivore-induced metabolomes of WT plants. Pairwise PERMANOVA of the UniFrac distance matrix. Pairwise differences between groups were tested using 5,000 unrestricted permutations. P values were calculated using upper-tail permutation tests and adjusted for multiple comparisons using the Benjamini–Hochberg method

	ctrl	Lp1	Lp2	Lp3	Mp1	Mp2	Mp3	Px1	Px2	Px3	SI1	SI2	SI3
ctrl	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Lp1	0.0006	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Lp2	0.0006	0.0010	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Lp3	0.0006	0.0006	0.0069	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Mp1	0.0006	0.0006	0.0006	0.0006	NA	NA	NA	NA	NA	NA	NA	NA	NA
Mp2	0.0006	0.0006	0.0006	0.0007	0.1369	NA	NA	NA	NA	NA	NA	NA	NA
Mp3	0.0006	0.0006	0.0006	0.0007	0.0120	0.0093	NA	NA	NA	NA	NA	NA	NA
Px1	0.0006	0.0007	0.0007	0.0006	0.0006	0.0006	0.0006	NA	NA	NA	NA	NA	NA
Px2	0.0006	0.0006	0.0006	0.0006	0.0006	0.0006	0.0006	0.0878	NA	NA	NA	NA	NA
Px3	0.0007	0.0006	0.0006	0.0006	0.0006	0.0007	0.0007	0.0083	0.1874	NA	NA	NA	NA
SI1	0.0006	0.0006	0.0006	0.0006	0.0006	0.0006	0.0006	0.0010	0.0006	0.0046	NA	NA	NA
SI2	0.0006	0.0006	0.0006	0.0006	0.0006	0.0006	0.0007	0.0006	0.0006	0.0019	0.0308	NA	NA
SI3	0.0007	0.0006	0.0006	0.0006	0.0006	0.0006	0.0006	0.0006	0.0007	0.0017	0.0057	0.0630	NA

Supplementary Table 2.

p values of pairwise PERMANOVA between phytohormone-induced metabolomes of WT plants. Pairwise PERMANOVA of the UniFrac distance matrix. Pairwise differences between groups were tested using 5,000 unrestricted permutations. P values were calculated using upper-tail permutation tests and adjusted for multiple comparisons using the Benjamini–Hochberg method

	MeJA 0.1 μ M	MeJA 0.5 μ M	MeJA 1 μ M	MeSA 0.1 μ M	MeSA 0.5 μ M	MeSA 1 μ M	Mock
MeJA 0.1 μ M	NA	NA	NA	NA	NA	NA	NA
MeJA 0.5 μ M	0.0031	NA	NA	NA	NA	NA	NA
MeJA 1 μ M	0.0031	0.0050	NA	NA	NA	NA	NA
MeSA 0.1 μ M	0.0031	0.0031	0.0031	NA	NA	NA	NA
MeSA 0.5 μ M	0.0031	0.0031	0.0031	0.0031	NA	NA	NA
MeSA 1 μ M	0.0031	0.0031	0.0031	0.0036	0.0031	NA	NA
Mock	0.0031	0.0031	0.0031	0.0031	0.0031	0.0031	NA

Supplementary Table 3.

p values of pairwise PERMANOVA between herbivore-induced metabolomes of *myc2/3/4* plants. Pairwise PERMANOVA of the UniFrac distance matrix. Pairwise differences between groups were tested using 5,000 unrestricted permutations. P values were calculated using upper-tail permutation tests and adjusted for multiple comparisons using the Benjamini–Hochberg method

	ctrl	Lp1	Lp2	Lp3	Mp1	Mp2	Mp3	Px1	Px2	Px3	SI1	SI2	SI3
ctrl	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Lp1	0.0006	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Lp2	0.0006	0.0023	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Lp3	0.0006	0.0008	0.2544	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Mp1	0.0006	0.0006	0.0006	0.0006	NA	NA	NA	NA	NA	NA	NA	NA	NA
Mp2	0.0006	0.0010	0.0024	0.0024	0.0016	NA	NA	NA	NA	NA	NA	NA	NA
Mp3	0.0006	0.0006	0.0014	0.0014	0.0008	0.6217	NA	NA	NA	NA	NA	NA	NA
Px1	0.0006	0.0006	0.0006	0.0006	0.0006	0.0006	0.0006	NA	NA	NA	NA	NA	NA
Px2	0.0006	0.0012	0.0006	0.0006	0.0006	0.0008	0.0008	0.0076	NA	NA	NA	NA	NA
Px3	0.0006	0.0008	0.0008	0.0006	0.0006	0.0010	0.0006	0.0016	0.0734	NA	NA	NA	NA
SI1	0.0006	0.0006	0.0006	0.0006	0.0006	0.0006	0.0006	0.0006	0.0006	0.0006	NA	NA	NA
SI2	0.0006	0.0006	0.0006	0.0006	0.0006	0.0008	0.0006	0.0012	0.0006	0.0008	0.0192	NA	NA
SI3	0.0006	0.0008	0.0006	0.0006	0.0006	0.0006	0.0006	0.0006	0.0008	0.0006	0.0103	0.0907	NA

Supplementary Table 4.

p values of pairwise PERMANOVA between herbivore-induced metabolomes of *npr1* plants. Pairwise PERMANOVA of the UniFrac distance matrix. Pairwise differences between groups were tested using 5,000 unrestricted permutations. P values were calculated using upper-tail permutation tests and adjusted for multiple comparisons using the Benjamini–Hochberg method

	ctrl	Lp1	Lp2	Lp3	Mp1	Mp2	Mp3	Px1	Px2	Px3	SI1	SI2	SI3
ctrl	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Lp1	0.0005	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Lp2	0.0005	0.0408	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Lp3	0.0005	0.0007	0.0559	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Mp1	0.0012	0.0007	0.0006	0.0005	NA	NA	NA	NA	NA	NA	NA	NA	NA
Mp2	0.0007	0.0005	0.0005	0.0007	0.3419	NA	NA	NA	NA	NA	NA	NA	NA
Mp3	0.0005	0.0006	0.0005	0.0005	0.0040	0.1533	NA	NA	NA	NA	NA	NA	NA
Px1	0.0005	0.0007	0.0007	0.0007	0.0010	0.0014	0.0005	NA	NA	NA	NA	NA	NA
Px2	0.0005	0.0006	0.0005	0.0005	0.0006	0.0007	0.0006	0.0016	NA	NA	NA	NA	NA
Px3	0.0007	0.0005	0.0006	0.0005	0.0006	0.0006	0.0006	0.0630	0.3951	NA	NA	NA	NA
SI1	0.0007	0.0006	0.0006	0.0005	0.0006	0.0006	0.0005	0.0006	0.0006	0.0022	NA	NA	NA
SI2	0.0005	0.0007	0.0007	0.0006	0.0005	0.0005	0.0005	0.0005	0.0005	0.0012	0.0005	NA	NA
SI3	0.0006	0.0006	0.0006	0.0005	0.0005	0.0006	0.0007	0.0006	0.0005	0.0005	0.0005	0.0288	NA

Supplementary Table 5.

p values of pairwise PERMANOVA between herbivore-induced metabolomes of *bak1-5* plants. Pairwise PERMANOVA of the UniFrac distance matrix. Pairwise differences between groups were tested using 5,000 unrestricted permutations. P values were calculated using upper-tail permutation tests and adjusted for multiple comparisons using the Benjamini–Hochberg method

	ctrl	Lp1	Lp2	Lp3	Mp1	Mp2	Mp3	Px1	Px2	Px3	SI1	SI2	SI3
ctrl	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Lp1	0.0018	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Lp2	0.0008	0.0007	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Lp3	0.0007	0.0007	0.2348	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Mp1	0.0007	0.0007	0.0007	0.0007	NA	NA	NA	NA	NA	NA	NA	NA	NA
Mp2	0.0008	0.0010	0.0007	0.0007	0.0061	NA	NA	NA	NA	NA	NA	NA	NA
Mp3	0.0008	0.0007	0.0007	0.0007	0.0007	0.0008	NA	NA	NA	NA	NA	NA	NA
Px1	0.0007	0.0007	0.0007	0.0007	0.0008	0.0026	0.0007	NA	NA	NA	NA	NA	NA
Px2	0.0007	0.0007	0.0012	0.0007	0.0008	0.0007	0.0008	0.0088	NA	NA	NA	NA	NA
Px3	0.0007	0.0007	0.0007	0.0008	0.0007	0.0018	0.0007	0.1024	0.1130	NA	NA	NA	NA
SI1	0.0007	0.0007	0.0007	0.0007	0.0007	0.0007	0.0007	0.0008	0.0007	0.0007	NA	NA	NA
SI2	0.0007	0.0008	0.0007	0.0007	0.0007	0.0008	0.0007	0.0007	0.0007	0.0007	0.0204	NA	NA
SI3	0.0014	0.0007	0.0010	0.0012	0.0008	0.0008	0.0010	0.0014	0.0012	0.0026	0.0008	0.0171	NA

Supplementary Table 6.

p values of pairwise PERMANOVA between herbivore-induced metabolomes of *sobir1* plants. Pairwise PERMANOVA of the UniFrac distance matrix. Pairwise differences between groups were tested using 5,000 unrestricted permutations. P values were calculated using upper-tail permutation tests and adjusted for multiple comparisons using the Benjamini–Hochberg method

	ctrl	Lp1	Lp2	Lp3	Mp1	Mp2	Mp3	Px1	Px2	Px3	SI1	SI2	SI3
ctrl	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Lp1	0.0006	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Lp2	0.0006	0.3186	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Lp3	0.0006	0.0022	0.0716	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Mp1	0.0010	0.0038	0.0006	0.0006	NA	NA	NA	NA	NA	NA	NA	NA	NA
Mp2	0.0006	0.0116	0.0034	0.0006	0.4721	NA	NA	NA	NA	NA	NA	NA	NA
Mp3	0.0006	0.0097	0.0040	0.0006	0.0141	0.0934	NA	NA	NA	NA	NA	NA	NA
Px1	0.0006	0.0008	0.0006	0.0006	0.0006	0.0006	0.0006	NA	NA	NA	NA	NA	NA
Px2	0.0006	0.0006	0.0006	0.0006	0.0006	0.0006	0.0006	0.0078	NA	NA	NA	NA	NA
Px3	0.0006	0.0006	0.0006	0.0006	0.0008	0.0008	0.0008	0.0015	0.1114	NA	NA	NA	NA
SI1	0.0006	0.0006	0.0006	0.0006	0.0006	0.0006	0.0006	0.0006	0.0006	0.0006	NA	NA	NA
SI2	0.0010	0.0006	0.0006	0.0008	0.0006	0.0006	0.0006	0.0006	0.0006	0.0006	0.0809	NA	NA
SI3	0.0006	0.0006	0.0008	0.0006	0.0008	0.0006	0.0006	0.0006	0.0006	0.0013	0.0006	0.0665	NA

Supplementary Method 1. Detailed description on network analysis.

This section details how the metabolite co-association network used in Figure 6 is constructed and interpreted. The network is used to identify metabolites that occupy central (hub) positions in the herbivore-induced metabolic response, and to test whether the phytohormones (JA/SA/ABA) act as such hubs.

To construct an association network among features, we estimated a partial-correlation network using a Gaussian graphical model (GGM). Assuming a multivariate Gaussian distribution with covariance matrix Σ and precision matrix $\Omega = \Sigma^{-1}$, the conditional associations are encoded in the off-diagonal elements of Ω . Specifically, $\Omega_{ij} = 0$ for $i \neq j$ indicates conditional independence between variables i and j given all remaining variables, whereas nonzero values indicate an association that is not fully explained by the remaining variables. Partial correlations were computed as $\rho_{ij} = -\Omega_{ij} / \sqrt{\Omega_{ii} \Omega_{jj}}$. Edges were defined from these partial correlations: an absent edge corresponds to $\rho_{ij} = 0$, whereas retained edges have nonzero ρ_{ij} values, with edge strength determined by their absolute magnitude. Unlike covariance- or marginal-correlation-based networks, which connect features based on their overall pairwise co-variation, the GGM-based partial-correlation network admits a regression-based interpretation. An edge between two features indicates that their residuals remain associated after each feature is regressed on all other measured features. Thus, the network represents conditional associations that are not explained by the remaining features.¹

For network estimation, graphical lasso regularization was applied to impose sparsity on the estimated precision matrix, so that weak conditional associations were set to zero and the network retained the stronger conditional-dependence patterns. The regularization path was fitted using the `huge` function in the `huge` package with `method = "glasso"` and `lambda = seq(2, 0.05, length.out = 20)`, after standardizing each variable to mean 0 and unit variance. The optimal regularization parameter within this path was selected using the `huge.select` function in the `huge` package with `criterion = "ebic"` and the default `ebic.gamma = 0.5`.² The partial correlations from the estimated Ω defined the weighted adjacency matrix of the undirected partial-correlation network as $W_{ij} = |\rho_{ij}|$ for $i \neq j$, otherwise $W_{ii} = 0$. Off-diagonal entries were assigned the corresponding absolute partial-correlation magnitude, whereas diagonal entries were set to zero. Absolute edge weights were used so that node-level measures reflected the magnitude of conditional associations regardless of sign.

The estimated network was then summarized using the following node centrality measures. Degree centrality was calculated from the binary support of the weighted adjacency matrix as $k_i = \sum_{j \neq i} I(W_{ij} > 0)$, where $I(\cdot)$ is the indicator function. It counts nonzero edges incident to node i and was computed using the degree function in the igraph package. This measure uses only edge presence and does not incorporate edge magnitude. Eigenvector centrality was defined as the elements of the principal eigenvector of the weighted adjacency matrix, satisfying $Wx = \lambda_{\max} x$, where x is the principal eigenvector and $\lambda_{\max}$ is the largest eigenvalue. It was computed using the `eigen_centrality` function in the igraph package with edge weights W_{ij} . This measure is larger for nodes connected to other highly central nodes. Because betweenness and closeness centralities rely on shortest-path calculations, edge weights were converted into edge lengths before computing these metrics. For each retained edge, the edge length was defined as $d_{ij} = 1 / W_{ij}$, so that stronger conditional associations corresponded to shorter distances. Entries with $W_{ij} = 0$ were treated as absent edges and were not assigned edge lengths. Betweenness centrality quantified how often a node lies on shortest paths between other node pairs and was calculated as $b_i = \sum_{s < t, s, t \neq i} [\sigma_{st}(i) / \sigma_{st}]$, where σ_{st} is the number of paths from s to t that achieve the minimum total edge length, using d_{ij} as the length of each retained edge, and $\sigma_{st}(i)$ is the number of those paths passing through node i . The normalized score was computed using the betweenness function in the igraph package, with these edge lengths and `normalized = TRUE`. For closeness centrality, let s_{ij} denote the shortest-path distance between nodes i and j , defined as the minimum total edge length over all paths connecting them. If no path connects the two nodes, s_{ij} was treated as infinite for that pair. For connected graphs, closeness was calculated as $c_i = (n - 1) / [\sum_{j \neq i} s_{ij}]$. For disconnected graphs, harmonic closeness was used as $h_i = [\sum_{j \neq i} 1/s_{ij}] / (n - 1)$, with unreachable node pairs contributing zero. These shortest-path distances were computed using the `distances` function in the igraph package. A larger closeness or harmonic closeness value therefore indicates that a node is closer to the rest of the network under this edge-length definition. For all node-level centrality metrics reported here, higher values indicate greater centrality under the corresponding metric.

References

1. Epskamp, S. & Fried, E. I. A tutorial on regularized partial correlation networks. *Psychol Methods* **23**, 617–634 (2018).
2. Foygel, R. & Drton, M. Extended Bayesian Information Criteria for Gaussian Graphical Models. in *Advances in Neural Information Processing Systems* vol. 23 (Curran Associates, Inc., 2010).