

## Titles of supplementary files

**Figure S1. Rarefaction curves of metabarcoding sequences.**

**Figure S2. Principal coordinate analysis without INO at the tree stage.** Bray-Curtis dissimilarities between samples were used for these analyses. Each dot corresponds to one sample. Labels of plant species are displayed at the barycenter of dots. CYC: *Cyclophyllum barbatum*, IXO: *Ixora moorensis*, MIC: *Miconia calvenscens*, SPA: *Spathodea campanulata*, SYZ: *Syzygium malaccense*.

**Figure S3. Maximum-likelihood phylogenetic tree of dominant bacterial ASV of MIC trees.** The tree was rooted using an archaeon. Numbers are ultrafast bootstraps (%) reflecting clade support. The ASV used in this figure were the 10 dominant ASV of MIC at the tree stage. MIC: *Miconia calvenscens*. ASV: amplicon sequence variant.

**Figure S4. Examples of spectral similarity networks of terpenes biomarkers associated with their respective boxplot and annotation.** MIC: *Miconia calvenscens*.

**Table S1. Metadata and metabarcoding denoising.**

**Table S2. Bacterial abundances and annotations.** CYC: *Cyclophyllum barbatum*, INO: *Inocarpus fagifer*, IXO: *Ixora moorensis*, MIC: *Miconia calvenscens*, SPA: *Spathodea campanulata*, SYZ: *Syzygium malaccense*. S: seedling. T: tree. ASV: amplicon sequence variant.

**Table S3. Microeukaryotes abundances and annotations.** CYC: *Cyclophyllum barbatum*, INO: *Inocarpus fagifer*, IXO: *Ixora moorensis*, MIC: *Miconia calvenscens*, SPA: *Spathodea campanulata*, SYZ: *Syzygium malaccense*. S: seedling. T: tree. ASV: amplicon sequence variant.

**Table S4. Metazoan abundances and annotations.** CYC: *Cyclophyllum barbatum*, INO: *Inocarpus fagifer*, IXO: *Ixora moorensis*, MIC: *Miconia calvenscens*, SPA: *Spathodea campanulata*, SYZ: *Syzygium malaccense*. S: seedling. T: tree. ASV: amplicon sequence variant.

**Table S5. Metabolites identified with the positive ionization mode.** CYC: *Cyclophyllum barbatum*, INO: *Inocarpus fagifer*, IXO: *Ixora moorensis*, MIC: *Miconia calvenscens*, SPA: *Spathodea campanulata*, SYZ: *Syzygium malaccense*. S: seedling. T: tree. R: root.

**Table S6. Metabolites identified with the negative ionization mode.** CYC: *Cyclophyllum barbatum*, INO: *Inocarpus fagifer*, IXO: *Ixora mooreensis*, MIC: *Miconia calvenscens*, SPA: *Spathodea campanulata*, SYZ: *Syzygium malaccense*. S: seedling. T: tree. R: root.

**Table S7. Alpha diversity metrics.** CYC: *Cyclophyllum barbatum*, INO: *Inocarpus fagifer*, IXO: *Ixora mooreensis*, MIC: *Miconia calvenscens*, SPA: *Spathodea campanulata*, SYZ: *Syzygium malaccense*. S: seedling. T: tree.

**Table S8. Significant associations between plant species and soil taxa.** CYC: *Cyclophyllum barbatum*, INO: *Inocarpus fagifer*, IXO: *Ixora mooreensis*, MIC: *Miconia calvenscens*, SPA: *Spathodea campanulata*, SYZ: *Syzygium malaccense*. 1: presence of the taxa for the corresponding plant species. 0: absence. ASV: amplicon sequence variant.

**Table S9. Metabolite annotations.**