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GENUS-SPECIFIC METABOLIC SIGNATURES IN ORCHIDACEAE REVEALED BY LC-HRMS/MS AND MULTIVARIATE STATISTICAL ANALYSIS

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Untargeted metabolomics based on HPLC-HRMS/MS was applied to discriminate species from three Orchidaceae genera (*Vanda*, *Laelia*, and *Cymbidium*) and to identify genus-specific metabolic markers. A total of 28 samples were analyzed using a methanol-based extraction followed by SPE cleanup and LC-HRMS/MS analysis. Data processing and metabolite annotation were performed using molecular networking workflows (GNPS) and multivariate statistical analysis. From the dereplication of molecular features, 61 secondary metabolites were putatively annotated, encompassing flavonoids, terpenes, alkaloids, phenolic acids, lignans, stilbenes, and quinones, alongside a wide range of primary metabolites such as amino acids and sugars. Among secondary metabolites, flavonoids emerged as the most abundant and taxonomically informative class, with 19 structurally characterized compounds. Distinct distribution patterns were observed: *Laelia* exhibited the highest flavonoid diversity, including isovitexin and apigenin 6,8-digalactoside as dominant compounds. *Cymbidium* showed high levels of rutin and phenolic acids such as 3-(2-hydroxyphenyl)propionic acid, while *Vanda* displayed the lowest flavonoid abundance but a higher content of quinones and phenolic acids, suggesting a different metabolic specialization. Terpenoids were the most abundant class overall, particularly enriched in *Cymbidium* and *Laelia*, consistent with their biosynthetic versatility. Chromenones such as 7-hydroxy-4,8-dimethylchromen-2-one and anthraquinones like alizarin were also identified, with structural validation based on MS/MS fragmentation and GNPS spectral matches. Lignans and glycosylated derivatives, including (+)-syringaresinol β-D-glucoside, were preferentially found in *Laelia*, indicating potential chemophenetic significance. Multivariate analysis (PCA and PLS-DA) revealed clear clustering of samples according to genus, with specific metabolites driving the separation. Chemometric loading plots identified isovitexin, rutin, syringic acid, sinapic acid, and alizarin as major discriminators. These compounds may serve as putative chemotaxonomic markers for genus-level identification within Orchidaceae. Furthermore, observed metabolite patterns suggest that shikimate and phenylpropanoid pathways are central to the secondary metabolism of these genera, supporting the use of metabolomics in understanding orchid chemodiversity and taxonomy.

Keywords: *HRMS-based untargeted metabolomics, chemodiversity, terpenoids, flavonoids, chemometric*

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