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ATR-FTIR spectral fingerprinting and Chemometric classification of *Labisia pumila* varieties with exploratory screening of herbal products

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Abstract

Labisia pumila (syn. *Marantodes pumilum*), an important medicinal herb in Southeast Asia, exhibits compositional variability that complicates authentication of raw materials and related herbal products. In this study, attenuated total reflectance-Fourier transform infrared (ATR-FTIR) spectroscopy combined with chemometric analysis was applied as a rapid and non-destructive approach for differentiating authenticated cultivated *L. pumila* var. *alata* and var. *pumila* materials, and plant parts, with exploratory screening of related commercial herbal medicinal products (HMPs). A total of 310 ATR-FTIR technical replicate spectra were acquired from authenticated raw materials collected from multiple locations in Peninsular Malaysia and from solid commercial HMP contents. The fingerprint region of 1646–720 cm^{-1} provided the most informative spectral variation for sample discrimination. Principal component analysis (PCA), hierarchical cluster analysis (HCA), and partial least squares-discriminant analysis (PLS-DA) were used to evaluate spectral classification. PCA and HCA supported separation between *L. pumila* var. *alata* and var. *pumila* based on discriminative spectral features in the fingerprint region, while PCA additionally revealed clustering patterns associated with leaf and stem-root tissues. The final PLS-DA model, developed using the 273-variable fingerprint-region subset (1646–720 cm^{-1}) of the 490 VIP-selected variables from Savitzky–Golay first-derivative spectra, classified authenticated cultivated *L. pumila* var. *alata* and var. *pumila* raw materials based on their ATR-FTIR spectral fingerprints ($R^2Y = 0.894$, $Q^2 = 0.894$). Additional grouped leave-one-source-material-out validation correctly classified all 120 held-out spectra and all 12 cultivated source materials, while Y-randomization testing supported that the observed class separation was unlikely to be due to random class assignment. Commercial HMPs were subsequently projected onto the calibrated model as an exploratory prediction set to assess potential applicability to market samples. These findings demonstrate that ATR-FTIR spectral fingerprinting, combined with chemometric analysis, provides a cultivated-reference screening workflow for differentiating medicinally relevant *L. pumila* varieties and plant parts, with potential application in exploratory screening of commercial HMPs. © 2026 Elsevier B.V.

Author keywords

ATR-FTIR spectroscopy; Chemometrics; Herbal medicinal products; *Labisia pumila*; PLS-DA; Spectral fingerprinting

Indexed keywords

Engineering controlled terms

Cultivation; Discriminant analysis; Hierarchical clustering; Hierarchical systems; Materials testing; Palmprint recognition; Plant extracts; Principal component analysis; Screening; Source separation; Spectrum analysis; Supersaturation; Value engineering

Engineering uncontrolled terms

Attenuated total reflectance Fourier transform infrared; Attenuated total reflectance Fourier transform infrared spectroscopy; Chemometrics; Herbal medicinal product; Infrared spectral; Labisia pumila; Medicinal products; Partial least squares discriminant analyses (PLSDA); Principal-component analysis; Spectral fingerprinting

Engineering main heading

Fourier transform infrared spectroscopy

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