

Discrimination of three Pegaga (*Centella*) varieties and determination of growth-lighting effects on metabolites content based on chemometry of ^1H nuclear magnetic resonance spectroscopy.

ABSTRACT

The metabolites of three species of Apiaceae, also known as Pegaga, were analyzed utilizing ^1H NMR spectroscopy and multivariate data analysis. Principal component analysis (PCA) and hierarchical cluster analysis (HCA) resolved the species, *Centella asiatica*, *Hydrocotyle bonariensis*, and *Hydrocotyle sibthorpioides*, into three clusters. The saponins, asiaticoside and madecassoside, along with chlorogenic acids were the metabolites that contributed most to the separation. Furthermore, the effects of growth-lighting condition to metabolite contents were also investigated. The extracts of *C. asiatica* grown in full-day light exposure exhibited a stronger radical scavenging activity and contained more triterpenes (asiaticoside and madecassoside), flavonoids, and chlorogenic acids as compared to plants grown in 50% shade. This study established the potential of using a combination of ^1H NMR spectroscopy and multivariate data analyses in differentiating three closely related species and the effects of growth lighting, based on their metabolite contents and identification of the markers contributing to their differences.

Keyword: Pegaga varieties; Growth-lighting effects; Metabolites content; Chemometry; ^1H Nuclear Magnetic Resonance.