Ⅲ-4

UPLC/Q-TOF MS를 이용한 고본의 패턴 분석

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Pattern Recognition Analysis of *Angelica tenuissima* Nakai using UPLC/Q-TOF MS-Based Metabolite Profiling

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Objectives

Ultraperformance liquid chromatography/quadrupole time-of-flight mass spectrometry (UPLC/Q-TOF MS) technique applied to this metabolic profiling is a powerful tool due to its higher sensitivity, resolution, and speed compared to conventional HPLC technique.

In this study, we investigated pattern recognition analysis of *Angelica tenuissima* Nakai using UPLC/Q-TOF MS. In addition, we compared the pattern of *A. tenuissima* with those of *Ligusticum jeholense* Nakai, *Cnidium officinale* Makino, and *Angelica gigas* Nakai, which are confused in the use of *A. tenuissima* with its similarities in phenotype and constituents.

Materials and Methods

○ Materials

Each of the powdered *A. tenuissima*, *L. jeholense*, *C. officinale*, and *A. gigas* was extracted with 70% EtOH, filtered, and stored at -20℃ until analyzed.

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○ Methods

UPLC was performed using a Waters ACQUITY UPLC™system (Waters Corp., MA, USA), and mass spectrometry was performed using Q-TOF Micro mass detector (Waters, Manchester, UK). All ESI negative spectral data were processed using MarkerLynx (Waters, Manchester, UK) and R version 2.6.1 (R Foundation for Statistical Computing, Vienna, Austria) for multivariate analysis.

Results

UPLC/Q-TOF MS-based metabolomics allowed the direct detection of various metabolites in *A. tenuissima*. Acquired data were then subsequently applied to principal component analysis (PCA) and hierarchical clustering analysis (HCA). PCA score plot (Fig. 1) and HCA dendrogram (Fig. 2) showed clear separation among origins of *A. tenuissima*, *L. jeholense*, *C. officinale*, and *A. gigas* as a result. These results suggest that the developed metabolomics tool with UPLC/Q-TOF MS successfully identify and classify all tested samples according to their origins.

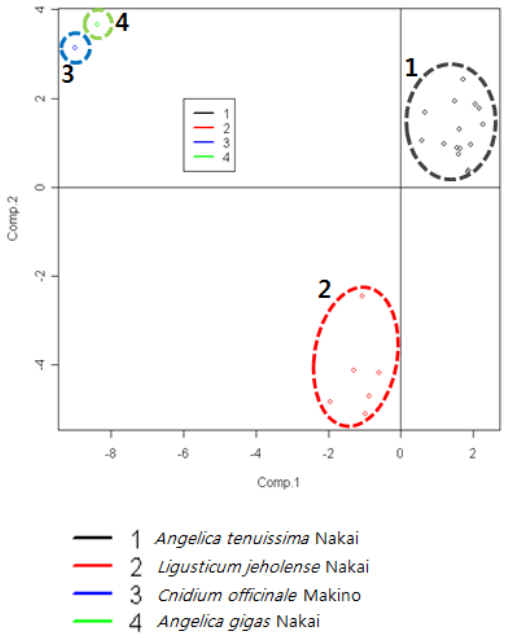

Fig.1. PCA score plot.

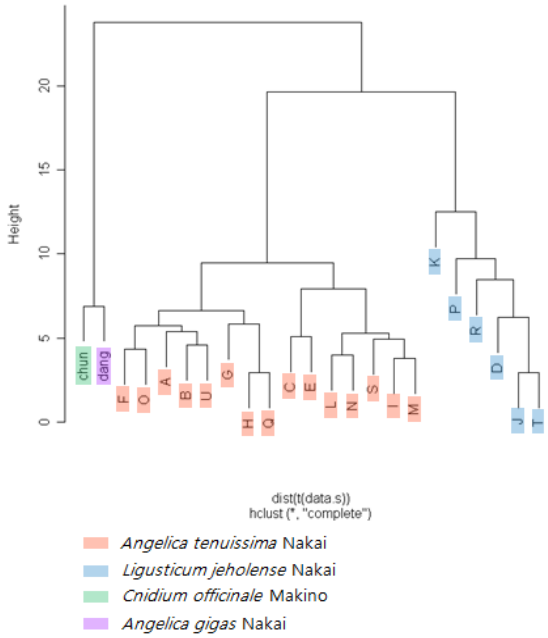

Fig.2. HCA dendrogram.