



## 基于气质联用的款冬花蕾动态发育代谢组学特征分析

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**中文摘要:**目的: 采用气相色谱-质谱法(GC-MS)结合代谢组学分析技术明确不同发育阶段款冬花蕾的代谢组学特征。方法: 对款冬花5个不同发育阶段药材进行两相溶剂提取, 得到极性 和非极性部分, 分别对其进行GC-MS 测定。代谢产物的结构指认通过NIST 数据库检索和对照品对照确定, 将数据预处理后导入SIMCA-P软件进行多元统计分析。结果: 共鉴定了54个代谢产物, 包括35个极性化合物和19个非极性化合物, 主成分分析(PCA)结果显示5个阶段的款冬花蕾样品能较为明显的分开, 且呈动态变化趋势, 与传统采收期12月样品相比, 10月和11月的花蕾样品与12月相距较近, 说明这3个阶段的代谢组组成接近, 而9月和3月的样品则距离较远, 说明这2个时间点的样品化学差异较大。通过对部分特征代谢物相对含量进行比较, 发现款冬花蕾发育过程中, 脯氨酸、赖氨酸和亚油酸在发育初期含量较低, 中期升至最高, 在开花后又急剧下降; 苹果酸和柠檬酸在中期含量较低; 蔗糖的含量逐渐降低, 开花后降至最低。结论: 发育初期和开花后与传统采收期款冬花样品的化学差异较大, 为其不能入药提供了科学依据, 也为款冬花合理采收期的确定及其药效物质基础研究奠定了基础。

中文关键词: 款冬 花蕾 发育 GC-MS 代谢组学

## Metabolomic study of flower buds of *Tussilago farfara* in different development stages by GC-MS

**Abstract: Objective:** Plant metabolomics combined with GC-MS was used to investigate metabolic fingerprinting of *Tussilago farfara* at different growth stages. **Method:** Dried Samples were extracted by two-phase solvent system to obtain polar and nonpolar parts, which were subjected to GC-MS analysis. Metabolites were identified by NIST data base search and comparison with the authentic standards. The data were introduced into SIMCA-P 11.0 software package for multivariate analysis after pretreatment. **Result:** Fifty-four metabolites were identified, including 35 polar metabolites and 19 nonpolar compounds. The score plot for PCA showed clear separation of the different development stages of flower buds of *T. farfara*, showing a trend of gradual change. Samples of October, November, December were in close proximity on the plot, indicating that the metabolome of these three periods was similar, samples from September (early development) and March (after flowering) were far away, showing big chemical differences. Content comparison results of some representative metabolites reveals that, the content of proline, lysine and linoleic acid increased gradually to the highest in the medium term, but sharply decreased to the lowest after flowering; the content of malic acid and citric acid were the lowest in the medium term; sucrose content decreased gradually, and then reached the lowest level after blooming. **Conclusion:** It is obvious that metabolites of the early development and flowering stage were quite different with those of the traditional harvest time, suggesting that they can not be used as traditional medicine. This study will provide a research basis for harvest time determination and bioactive compounds of *T. farfara*.

**keywords:** *Tussilago farfara* flower buds development GC-MS metabolomics

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