

研究报告

# HPLC/ESI-MS法鉴定半枝莲乙酸乙酯组分中黄酮苷元类化合物

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**摘要** 利用正离子模式电喷雾质谱研究了包括正黄酮、异黄酮、二氢黄酮、异二氢黄酮和黄酮醇在内的5个黄酮亚类苷元的质谱断裂碎片, 并得到了能够区别鉴定这5类黄酮苷元的特征碎片离子。其中, 2个CO的连续丢失可以看作异黄酮的特征断裂,  $[^{0,4}B-H_2O+H]^+$ 是二氢黄酮的特征碎片离子, 黄酮醇和异二氢黄酮则主要发生0, 2键和2, 3键的断裂, 分别形成特征的 $^{0,2}A^+$ 和 $^{2, 3}B^+$ 碎片离子。在此基础上, 利用高效液相色谱与电喷雾质谱联用技术对半枝莲乙酸乙酯组分中的化合物进行研究, 确定了异红花素(isocarthamidin)、印黄芩素(scutellarin)、木樨草素(luteolin)、柚皮素(naringenin)、4'-羟基汉黄芩素(4'-hydroxy-wogonin)和芹菜素(apigenin)6个黄酮苷元, 并结合紫外光谱信息和质谱碎片信息, 对另外6个黄酮苷元类化合物进行初步的结构推断。

**关键词** [半枝莲](#) [黄酮苷元](#) [高效液相色谱](#) [电喷雾质谱](#)

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## Identification of Flavonoid Aglycones in Ethyl Acetate Multi-Components of *Scutellaria barbata* D. Don by HPLC/ESI-MS

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**Abstract** The flavonoid aglycones in ethyl acetate multi-components of *Scutellaria barbata* D. Don were identified by high performance liquid chromatography/positive electrospray ionization-mass spectrometry (HPLC/ESI-MS). Because the fragmentation behaviors of the flavonoid aglycones were crucial for the identification of unknown flavonoid aglycones, the characteristic MS fragments of five subclasses of flavonoid aglycones were initially studied using positive ion ESI-MS. The results indicate that the consequential loss of two CO molecules can be regarded as the diagnostic fragmentation pathway of isoflavone.  $^{0,2}A^+$  and  $^{2, 3}B^+$  fragments originated from the cleavage of C—C bonds of C-ring at positions 0/2 and 2/3 are the characteristic fragments of flavonol and isoflavanone respectively, and  $[^{0,4}B-H_2O+H]^+$  can be used to identify the flavanones. Based on these characteristic fragments, six flavonoids including isocarthamidin, scutellarin, luteolin, naringenin, 4'-hydroxy-wogonin and apigenin are identified unambiguously. Then, combined with the chromatographic retention time and UV spectra, another six compounds are identified tentatively.

**Key words** [Scutellaria barbata](#) D. Don [flavonoid aglycones](#) [HPLC](#) [ESI-MS](#)

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