

研究报告

# 水飞蓟宾的负离子电喷雾离子阱质谱研究

韩建平<sup>1</sup>; 李伟<sup>1, 2</sup>; 张超<sup>1</sup>; 王宏志<sup>1</sup>; 高钧<sup>1</sup>; 刘昌孝<sup>2, 3</sup>

1. 天津天士力集团有限公司, 天津 300402
2. 天津大学化工学院, 天津 300072
3. 天津药物研究院, 天津药代动力学与药效动力学省部共建国家重点实验室, 天津 300193

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**摘要** 采用电喷雾离子阱 (ESI-MS) 质谱技术对水飞蓟宾的结构和裂解途径进行研究。采用ESI-MS获得了  $m/z$  481[M-H]<sup>-</sup>, 采用ESI-MS<sup>2</sup>获得了  $m/z$  453、 $m/z$  301等碎片离子。发现ESI-MS<sup>2</sup>质谱生成A环和B环C—O—C键断裂的碎片, 并对  $m/z$  453、 $m/z$  301特征碎片离子进行ESI-MS<sup>3</sup>质谱研究, 归属了其重要特征碎片离子, 分析和讨论了该化合物的结构和质谱特征。

**关键词** [水飞蓟宾](#) [电喷雾离子阱质谱](#) [裂解途径](#)

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## Study on Silybin in Negative Mode by Ion Trap Mass Spectrometry

HAN Jian-ping<sup>1</sup>; LI Wei<sup>1, 2</sup>; ZHANG Chao<sup>1</sup>; WANG Hong-zhi<sup>1</sup>; GAO Jun<sup>1</sup>; LIU Chang-xiao<sup>2, 3</sup>

1. Tasly R&D Institute, Tianjin Tasly Group Co. Ltd. , Tianjin 300402, China;
2. School of Chemical Engineering and Technology, Tianjin University, Tianjin 300072, China;
3. Tianjin State Key Laboratory of Pharmacokinetics and Pharmacodynamics, Tianjin institute of Pharmaceutical Research, Tianjin 300193, China

**Abstract** The structure and fragmentation pathway of silybin were elucidated by electron spray ionization mass spectrometry (ESI-MS) . Quasi-molecular ion peak  $m/z$  481 [M-H]<sup>-</sup> was detected by ESI-MS, and the ions of  $m/z$  453 and  $m/z$  301 were detected by ESI-MS<sup>2</sup>. The fragment routes of characteristic were discussed on the basis of ESI mass spectra. The full scan MS<sup>2</sup> spectra of silybin gave characteristic fragment ions formed through cleavage of the C—O—C bond at A-ring and B-ring. The full scan MS<sup>3</sup> spectra of fragment  $m/z$  453,  $m/z$  301 was obtained by ion trap mass spectrometry. The characteristic fragmentation was used to prove the structure of  $m/z$  453,  $m/z$  301.

**Key words** [silybin](#) [electron spray ionization-ion trap mass spectrometry](#) [fragmentation pathway](#)

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