



Characterization of Metabolites in Rat after Administration of Danshensu by Liquid Chromatography-tandem Mass Spectrometry

Shuming LI ^{1,2}, Xiangyang WANG ², Wei LI ², Yang CHU ²,
Jiahua GUO ², Xiaohui MA ^{2,3} & Jin YANG ^{1*}

¹ Center of Drug Metabolism and Pharmacokinetics,
China Pharmaceutical University, Nanjing 210009, China

² Tasly R&D Institute, Tianjin Tasly Group Co., Ltd., Tianjin 300410, China

³ School of Pharmaceutical Science and Technology, Tianjin University, Tianjin 300072, China

SUMMARY. A method using liquid chromatography-electrospray ionization tandem mass spectrometry (LC-ESI-MS/MS) analysis was established for the identification of metabolites in rat urine and bile after oral administration and intravenous injection of Danshensu (3-(3,4-dihydroxyphenyl) lactic acid, DSS), a major bioactive phenolic acid in the roots of *Salvia miltiorrhiza*. Separation of rat metabolites by column chromatography was applied in this study. The results indicated that hydroxylation, sulfation, glycine conjugation and methylation were the major metabolic pathways of DSS. A total of six metabolites were identified in rat, among which the glycine conjugated metabolites was first reported in rat urine. Besides, the possible metabolic pathway was proposed. The established method was simple, sensitive and reliable for metabolites identification, contributing to our better understanding of their metabolism behavior *in vivo*.

KEY WORDS: Danshensu, Glycine conjugates, LC-MS/MS, Metabolites, *Salvia miltiorrhiza*.

* Author to whom correspondence should be addressed. E-mail: yjcpu@yahoo.cn