



高效液相色谱-质谱联用结合量子化学计算发现乌头碱一新水解产物

投稿时间: 2010-12-20 责任编辑: 丁广治 [点此下载全文](#)

引用本文: 谭鹏,刘永刚,关君,李飞,董玲,乔延江.高效液相色谱-质谱联用结合量子化学计算发现乌头碱一新水解产物[J].中国中药杂志,2011,36(15):2099.

DOI: 10.4268/cjmm201111519

摘要点击次数: 717

全文下载次数: 249

广告合作



作者中文名	作者英文名	单位中文名	单位英文名	E-Mail
谭鹏	TAN Peng	北京中医药大学,北京100102	Beijing University of Chinese Medicine, Beijing 100102, China	
刘永刚	LIU Yonggang	北京中医药大学,北京100102	Beijing University of Chinese Medicine, Beijing 100102, China	
关君	GUAN Jun	北京中医药大学,北京100102	Beijing University of Chinese Medicine, Beijing 100102, China	
李飞	LI Fei	北京中医药大学,北京100102	Beijing University of Chinese Medicine, Beijing 100102, China	
董玲	DONG Ling	北京中医药大学,北京100102	Beijing University of Chinese Medicine, Beijing 100102, China	
乔延江	QIAO Yanjiang	北京中医药大学,北京100102	Beijing University of Chinese Medicine, Beijing 100102, China	yjqiao@263.net

基金项目:国家自然科学基金项目(30901959);国家重点基础研究发展计划(973)项目(2009CB522800)

中文摘要:目的:高效液相色谱-质谱/质谱(HPLC-MSⁿ)结合量子化学计算发现乌头碱的新水解产物。方法:HPLC-MSⁿ方法采用梯度洗脱,质谱用正离子模式。采用密度泛函方法在B3LYP/6-31G(d)水平上,对可能的产物结构进行计算。结果:通过HPLC-MSⁿ的检测发现乌头碱水解产生分子离子峰为482的化合物,推测结构为脱水乌头原碱。量子化学计算结果只有C8和C15位发生消除反应的产物得到了最低能量构象,分析推测分子离子峰为482的化合物为C15位羰基的脱水乌头原碱。结论:首次发现乌头碱加热热水解生成脱水乌头原碱,推测了乌头碱水解的两条新水解途径。

中文关键词:HPLC-MSⁿ; 量子化学; 乌头碱; 脱水乌头原碱; 水解

Studies on new hydrolysate of aconitine using HPLC-MSⁿ and quantum chemistry calculation

Abstract:Objective: To study the new hydrolysate of aconitine using HPLC-MSⁿ and quantum chemistry calculation. Method: The HPLC method was applied in gradient elution program and the mass spectrometry was in positive ion mode. Geometries of the possible hydrolysates were optimized at DFT/6-31G(d) level. Result: The new hydrolysate was found and its protonated molecular ions was at *m/z* 482. The quantum chemistry calculation results show that the product of elimination reactions at C8 and C15 got the lowest energy conformation. The compound at *m/z* 482 was deduced to be the hydrolysate of carbonyl at C15. Conclusion: Delydration aconine was detected for the first time and the new hydrolysis pathways of aconitine in water were deduced.

keywords:HPLC-MSⁿ; quantum chemistry calculation; aconitine; hydrolysis aconine; hydrolysis

[查看全文](#) [查看/发表评论](#) [下载PDF阅读器](#)