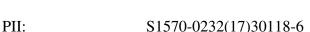
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Title: Using UHPLC Q-Trap/MS as a Complementary Technique to In-depth Mine UPLC Q-TOF/MS Data for Identifying Modified Nucleosides in Urine

Author: Zhiwei Lu Qing Wang Meiling Wang Shuang Fu Qingqing Zhang Zhixin Zhang Huizhen Zhao Yuehong Liu Zhenhai Huang Ziye Xie Honghong Yu Xiaoyan Gao



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Highlights

2 1. PBA extraction was more efficiently than the other solid phase extraction (HLB, MCX cartridges) and protein 3 precipitation methods for extraction of cis-diol-containing biomolecules in this study. 4 2. It was a powerful method to comprehensively identify urinary nucleosides by combining UPLC Q-TOF/MS 5 with UHPLC Q-Trap/MS. 6 3. Five urinary nucleosides were identified for the first time, including 4',5'-didehydro-5'-deoxyadenosine, 7 4',5'-didehydro-5'-deoxyinosine, isonicotinamide riboside, and 2 hypermodified nucleosides, peroxywybutosine 8 and hydroxywybutosine. This was the first discovery of nucleoside peroxide from human urine. 9 10 **Full Length Article** 11 Using UHPLC Q-Trap/MS as a Complementary Technique to In-depth Mine UPLC 12 Q-TOF/MS Data for Identifying Modified Nucleosides in Urine 13 Zhiwei Lu a, Qing Wang A, Meiling Wang, Shuang Fu, Qingqing Zhang, Zhixin Zhang, Huizhen Zhao, Yuehong 14 Liu, Zhenhai Huang, Ziye Xie, Honghong Yu, Xiaoyan Gao * 15 School of Chinese Pharmacy, Beijing University of Chinese Medicine, South of Wangjing Middle Ring Road, 16 Chaoyang District, Beijing 100102, P. R. China; luzhiwei5233@sina.com (Z. Lu); wangqing_0046@bucm.edu.cn 17 wangmeiling@bucm.edu.cn Wang); fushuang 5716@163.com Wang); (M. 18 zhangqingqing1826@bucm.edu.cn (Q. Zhang); zzxzxz2@163.com (Z. Zhang); zhaohuizhen_2013@126.com (H. 19 Zhao); liuyuehong@bucm.edu.cn (Y. Liu); huangzhenghai0108@163.com (Z. Huang); xieziye200527@sina.com 20 (Z. Xie); yuhonghong@bucm.edu.cn (H. Yu); gaoxiaoyan0913@sina.com (X. Gao) * 21

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Abbreviations: UPLC Q-TOF/MS: ultra-promance liquid chromatography quadrupole time-of-flight mass spectrometry; UHPLC Q-Trap/MS: ultra-high performance liquid chromatography coupled with hybrid triple quadrupole linear ion trap mass spectrometer; SPE: solid phase extraction; MRM-EPI: multiple reaction monitoring trigger enhanced product ion scan; NL: neutral loss scan; PBA: phenylboronic acid; HMDB: Human Metabolome Database; LC/MS: liquid chromatography coupled with mass spectrometer; HDMS: high definition mass spectrometry; HLB: hydrophilic-lipophilic balance; MCX: mixed-mode cation exchange; IDA: information-dependent acquisition; EIC: extracted ion chromatogram.

^a The first two authors contributed equally to this work.

^{*} Corresponding author at: School of Chinese Pharmacy, Beijing University of Chinese Medicine, South of Wangjing Middle Ring Road, Chaoyang District, Beijing 100102, P. R. China. Tel./Fax: + 86 10 84738618. E-mail address: gaoxiaoyan0913@sina.com (X. Gao).

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