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Authors: Qingqing Zhang, Mengqi Huo, Yanling Zhang, Yanjiang Qiao, Xiaoyan Gao

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A strategy to improve the identification reliability of the chemical constituents by high-resolution mass spectrometry-based isomer structure prediction combined with a quantitative structure retention relationship analysis: phthalide compounds in Chuanxiong as a test case

Qingqing Zhang [a, b], Mengqi Huo [a], Yanling Zhang [a], Yanjiang Qiao[a, *], Xiaoyan Gao[a, **]

[a] School of Chinese Materia Medica, Beijing University of Chinese Medicine, Beijing 102488, China

[b] School of Pharmacy, Hebei University of Chinese Medicine, Shijiazhuang 050200, China

Highlights:

1. The candidate structures of phthalide isomer were predicted by structure and MS data.
2. QSRR model was developed and used to calculate retention time of phthalides.
3. The reliability of isomer structures was improved by matching the rational candidate.
4. Twenty-six potential new phthalide compounds were characterized.

Abbreviations: EICs, extracted ion chromatograms. ESI, electrospray ionization; HRMS, high resolution mass spectrometry; HRMS-ISP, HRMS based isomer structure prediction; MLR, multiple linear regression; QSRR, quantitative structure retention relationship; RMS, root mean square; SD, standard deviations; TCM, traditional Chinese medicine; TIC, total ion chromatogram; UPLC Q-TOF/MS^{E}, ultra performance liquid chromatography coupled with quadrupole time of flight tandem mass spectrometry; VIF, variance inflation factor.

*: Corresponding author: Prof. Yanjiang Qiao, School of Chinese Materia Medica, Beijing University of Chinese Medicine, South of Yangguang Street, Fangshan District, Beijing 102488, P. R. China. Tel./fax: +86 01084738621

**: Corresponding author: Prof. Xiaoyan Gao, School of Chinese Materia Medica, Beijing University of Chinese Medicine, South of Yangguang Street, Fangshan District, Beijing 102488, P. R. China. Tel./fax: +86 01084738618

E-mail address: gaoxiaoyan@bucm.edu.cn (X. Gao), yjqiao@263.net (Y. Qiao)