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Rapid identification of anti-inflammatory active ingredients from Tumuxiang based on spectrum-effect relationship and natural products application solution with UNIFI

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Traditional Chinese medicines (TCMs) have been playing a very important role in health protection and disease control for thousands of years. However, the low efficiency of studying material basis of TCMs is still the bottleneck of restricting Chinese medicine modernization. Nowadays, the latest Waters natural products application solution with UNIFI based on the ultra performance liquid chromatography (ACQUITY UPLC®H-Class), a quadrupole time of flight mass spectromete (Xevo®G2-S QTOf MS) and UNIFI Traditional Medicine Library can offer a turn-key solution. This method integrates data acquisition, data processing and Traditional Medicine Library in a highly automated fashion and makes the chemical composition analysis become simple, effective, sequencing and the work efficiency is greatly improved. In this work, the fingerprint chromatograms of twenty-seven Tumuxiang (TMX) samples were established by UPLC-QTOf-MS technique. At the same time, the anti-inflammatory property of TMX was evaluated by inflammatory models of dimethylbenzene-induced ear vasodilatation. Then, the spectrum-efficacy model between UPLC fingerprints and anti-inflammatory activities was investigated by principal component regression (PCR) and partial least squares (PLS). Finally, automated detection and data filtering were performed using the UNIFITM software. The results indicated that 80 peaks were identified by UNIFI, and 53 characteristic peaks had close correlation with anti-inflammatory activities. The proposed strategy showed high sensitivity, resolution and fast speed, as a brand new solution for complex component analysis of TCMs was more suitable for revealing and identifying the bioactive constituents in TMX, which provided the scientific evidence to preliminarily clarify material basis of anti-inflammatory activities of TMX.

Biography

Fangdi Hu has completed his PhD from Lanzhou University and Post-doctoral studies from Shanghai University of Traditional Chinese Medicine. She is a Professor at the Department of Natural Medicinal Chemistry, School of Pharmacy, Lanzhou University. She is mainly engaged in the analysis of Traditional Chinese Medicine. She has published more than 25 papers in reputed journals.

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