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New MS network analysis pattern for the rapid identification of constituents from traditional Chinese medicine prescription Lishukang capsules in vitro and in vivo based on ultra-high-performance liquid chromatography combined with quadrupole time-of-flight mass spectrometry

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Abstract

Ultra-high-performance liquid chromatography combined with quadrupole time-of-flight mass spectrometry (UHPLC-Q-TOF-MS) has recently been widely used in qualitative analyses of traditional Chinese medicine (TCM) prescriptions. However, a poor understanding of detected mass spectral data has rendered data processing difficult and time-consuming. Efficient and widespread data analysis methods focused on identifying both phytochemical compounds and metabolites of TCM prescriptions have rarely been described. In this study, a new MS network analysis pattern that uses model drug Lishukang (LSK) capsules to accelerate the data processing of TCM preparations is developed. The MS network analysis pattern integrates intrinsic structural correlations of phytochemical compounds and structural information derived from mass spectrometry to identify the same types of compounds from a raw data stream. As a result, five MS networks of flavones and flavone glycosides, alkaloids, phenolic acids, saponins and benzylester glucosides in LSK are preliminarily established. 278 compounds, including 9 potential novel compounds are identified or tentatively assigned based on MS networks. Furthermore, 57 potential metabolites of LSK are identified in rat plasma, and potential metabolic pathways are investigated under the guidance of MS networks in vitro. The MS network analysis pattern serves as an integral solution for identifying phytochemical compounds and metabolites of TCM prescriptions. The investigations of LSK also provide essential data for its further