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Rapid discovery and identification of unknown compounds in the active fraction from *Xiao-Xu-Ming* decoction (AF-XXMD) by HPLC-HRMS and MTSF technique

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Xiao-Xu-Ming decoction (XXMD) is a traditional Chinese formula and first recorded in "Bei Ji Qian Jin Yao Fang". It has been widely used to treat stroke in China. The active fraction of XXMD (AF-XXMD) exhibits similar pharmacological effects to XXMD. In the present work, a new strategy of the rapid discovery and identification of AF-XXMD compounds was established using high-performance liquid chromatography with high resolution mass spectrometry (HPLC-HRMS) and the mass spectral tree similarity filter technique (MTSF). With the MTSF technique, structurally-related compounds were discovered and identified by comparing the similarity between their mass spectral trees and library compounds. A total of 3362 compounds were automatically detected by HPLC-HRMS, and a 68 compounds were finally identified in AF-XXMD. The identified compounds included 14 library compounds with authentic standards, 50 structurally-related compounds fished by the MTSF technique, and 4 structurally-unrelated compounds identified by the manual method. This study successfully applied the MTSF technique should be useful to the discovery and identification of compounds in Chinese prescription. In addition, the MTSF technique is a promising technique for the targeted phytochemical separation in the future.

Biography

Caihong Wang is pursuing her studies in the Pharmaceutical Analysis department of Institute of Materia Medica, Chinese Academy of Medical Sciences & Peking Union Medical College as a PhD student. She has published three papers in Chinese Chemical Letters, *Phytomedicine, Journal of Pharmaceutical and Biomedical Analysis* and has been taking part in many reputed conferences.

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