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## ACCEPTED MANUSCRIPT

A full solution for multi-component quantification-oriented quality assessment of herbal medicines, Chinese agarwood as a case

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## **Highlights**

- ◆ A qualified tool was configured for Q-markers-oriented quality control of HMs.
- ◆ Automated fraction collector was utilized to prepare pseudo-authentic compounds.
- ◆ RPLC-HILIC-tailored MRM was used to address the wide content and polarity ranges.
- ◆ RRCEC matching was proposed for identity consolidation.
- ◆ Simultaneous determination of 26 analytes was conducted for Chinese agarwood.

#### **Abstract**

The quality of herbal medicines (HMs) is the prerequisite for their pronounced therapeutic outcomes in clinic, and multi-component (also known as quality markers, Q-markers) quantification has been widely emphasized as a viable means for quality evaluation. Because of the chemical diversity, the quality control practices are extensively dampened by four principal technical bottlenecks, including the lack of authentic compounds, large polarity span, extensive concentration range, and signal misrecognition for those potential Q-markers. An attempt to promote the potential of LC–MS/MS is made herein to cope with those obstacles and Chinese agarwood was employed as a case study. Firstly, a home-made fraction collector was introduced to automatically fragment the entire extract into a panel of fractions-of-interest. Secondly, quantitative <sup>1</sup>H NMR was deployed to offset the LC–MS/MS potential towards in-depth chemical profiling each fraction, and those

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