RESULTS AND DISCUSSIONS (III)

A rapid and effective strategy was adopted for the identification of compounds from ZSS using Natural Product Application Solution with UNIFI (Figure 4). Step 1: Integrate the NAPAS with UNIFI TM library and an in-house chemical library for ZSS based on the literature. Step 2: Screen the target ingredients from the UPLC-MS profile data, which is automatically performed by UNIFI platform (Figure 5). Step 3: Verify the identified compounds in the initial results according to authentic reference materials and confirm by reference standards. Step 4: Based on the results, three different MS fragmentation patterns were established, as well as the retention time of reference compounds. This is followed by summarizing and proposing fragmentation rules for target components. Step 5: Screen for potential new components with similar MS fragmentation patterns, and design specific methods for unknown precursor ions of identified known compounds. This is followed by summarizing and proposing fragmentation patterns of compounds of interests. Step 6: summarize the materials base and rationally evaluate the quality of ZSS-TCM products.

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