Profiling and annotation of flavonoids using a product ion-dependent MSn data acquisition method on a Tribrid Orbitrap mass spectrometer

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1. Abstract

The untargeted profiling of flavonoids provides insights into their biological functions and potential health benefits for humans. However, comprehensive identification of flavonoids from real samples remains challenging because of the limited availability of authentic standards and the structural diversity of this class of compounds. Previous studies relied upon extensive expert knowledge about fragmentation rules, a priori knowledge of the structures of flavonoids, and simple MS2 based analyses that are often not sufficient for complete structural characterization. Here we present a new flavonoid profiling workflow that uses comprehensive fragment ion information from HCD MS-MS and higher order FTMSn for rapid flavonoid identification and quantitation on a Tribrid Orbitrap mass spectrometer.

As the proof of concept of the workflow, flavonoid extracts from different types of natural products were tested. A C18 column was used for flavonoid separation, and a modified Orbitrap Fusion™ Tribrid™ mass spectrometer was used for collecting HRAM MS and MSn (up to MS5) data. The collected data were processed using Mass Frontier 8.0 and Compound Discoverer™ 3.0 software. A novel structure ranking algorithm included in the Compound Discoverer 3.0 software was applied to the MS and MSn data for confident structure elucidation of the unknown flavonoids based on ChemSpider database and custom flavonoids database. The MSn data were critical, especially for the identification of flavonoid glycocnjugates.

2. Brief Summary

The new LC-MSn workflow enables improved throughput, identification coverage and confidence for flavonoids profiling experiments