AN INTEGRATED HIGH RESOLUTION MASS SPECTROMETRIC AND INFORMATICS APPROACH FOR THE RAPID IDENTIFICATION OF FLAVONOIDS IN PLANT EXTRACT

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Introduction

The identification and characterization of phenol compounds in plants and manufactured foods represent an important analytical issue, which has blossomed during the last decades. Currently, HPLC coupled to mass spectrometry by APCl or ESI source represents the most selective analytical technique for the identification and quantification of phenol compounds from plants and foods. Here we report an integrated approach based on high resolution MS analysis (orbitrap) and database utilization for the rapid identification of plant phenols. This approach is firstly validated by using a mixture of phenolic standards and then applied for the rapid identification of phenols from Angelica Keiskei extract.

Overview of the integrated strategy

The LC/UV/ESI-MS analysis represents the first step, which is performed by using an orbitrap as a MS analyzer thus to retrieve accurate monoisotopic mass and isotopic mass distribution of the unknown compounds. The monoisotopic mass is then searched in a database (db) of polyphenols and the output is a list of compounds (list 1), which is then filtered on the basis of the chemical class to which the unknown compound belongs, as determined on the basis of the UV-Vis spectrum and on the well established UV absorption bands of flavonoids. For each entry belonging to the filtered list (list 2), simulated MS/MS fragments are predicted using the Mass Frontier software and the values are compared with the experimental fragments. The compounds are then ranked on the basis of the matched predicted/experimental fragments and the hit compound at the top of the list identifies the unknown. Final confirmation is then achieved by comparing experimental and simulated isotopic patterns.

Table 1: The method was firstly validated by analyzing a mixture of standards belonging to different polyphenol classes (hydroxycinnamates, flavones, flavonols, flavanones, flavanols, isoflavonoids); Db searching, UV-Vis data and experimental and predicted MS/MS data for flavonoids and phenolic acid standards are reported in the Table.

Table 2: The method was then applied for the identification of flavonoids contained in an EtOH extract of Angelica keiskei.

Conclusions

The proposed approach represents a new, reliable and potent tool for a facile and rapid identification of plant polyphenols. Moreover, such an approach can be successfully used without a strong background in polyphenol/flavonoid chemistry and MS/MS fragmentation knowledge, thus to greatly facilitate the phytochemical characterization of plant extracts.

References: