Phenolic compounds profiled by FT-ICR MS in *Stryphnodendron obovatum* Benth hidroethanolic leaves extracts

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Abstract

Stryphnodendron obovatum is a Brazilian Cerrado tree which hydroethanolic leaves extracts was assessed by ultrahigh resolution mass spectrometry (FT-ICR MS). Besides the presence of tannins, characteristic of this plant genus, flavonoids, catechins were also detected.

Introduction

S obovatum is a Brazilian Cerrado tree, rich in tannins. *Stryphnodendron sp.* barks are used in folk medicine to treat gonorhea, hernia, diarrhea and bleeding wounds.[1] But there were few phytochemical and biologycal studies from their *S obovatum* leaves. So, we have decided to assess the main phenolic constituents of the *S. obovatum* hydroethanolic leaves extracts by ultrahigh resolution mass spectrometry (FT-ICR MS) for a better understanding of their phytochemistry. This method has been used this method for the fingerprinting characterization of plant extracts complex mixtures, since it would provide an elemental composition from accurate mass measurement and metabolite structures with high degrees of certainty without the need of standards for each metabolite, saving time of sample preparation steps or prior chromatographic separation method.[2]

Results e Discussion

The leaves of *S. obovatum* (Fabaceae) were collected at FCL- Unesp Assis in July 2010. 60 g were extracted by dynamic maceration with ethanol:water 70:30 v/v (1:10 plant/solvent ratio, 3x2h), at room temperature. After filtration, the extract was concentrated under reduced pressure providing hydroethanolic extract (SOHE). For the ESI-MS analysis, 2 µL of leaves extracts were dissolved in a MeOH/H_2O (1:1 v/v) containing NH_4OH 0,1% solution and injected in 7.2T LTQ FT Ultra mass spectrometer (Thermo Scientific, Bremen, Germany), equipped with a direct infusion electrospray ionization source (ESI) operating in the negative-ion mode.

SOHE showed phenolic acids, flavonoids and catechins. The compound of *m/z* 169 was assigned to the gallic acid. For syringic acid (*m/z* 197), the ESI (-)-MS/MS show the fragments of *m/z m/z* 135 (loss of CO_2) and with *m/z* 179 (loss of water molecule). Other compounds such those of *m/z* 289, 301 and 317 were characterized as catechin, quercetin, and myricetin, respectively. Catechin also displays the fragment of *m/z* 254, that represents a loss of acetyl group as described Perez-Magarino et al.[3] Characteristic fragmentations of quercetin are resulted from cleavage of ring B after RDA elimination, forming the fragment of *m/z* 179 and also by loss of a carbonyl group (fragment of *m/z* 151).[4] Myricetin also showed a characteristic fragmentation ion of *m/z* 179 as reported by Quyeb et al. [5]

Compounds of *m/z* 447 was assigned as quercetin derivatives. The ion of *m/z* 447 was assigned to quercetin-3-O-β–deoxipentose. The MS/MS data showed an aglycone frangment of *m/z* 301 due loss a sugar moiety of 146 Da and the fragment of *m/z* 271 typical of flavon-3-*O*-monoglycoside. [6] For the ion of *m/z* 463, the MS/MS experiment produced a deprotonated aglycone form myricetin, ion of *m/z* 317(loss of a sugar moiety of 146 units), indicating that compound is a myricetin monohexoside (myricetin 3-O-galactoside or myricetin 3-O-glucoside).[7]

Epigallocatechin (m/z 305) yielded the fragment ions of *m/z* 125 and 179, which was consistent with the previous report.[8] Epigallocatechin dimer (*m/z* 609) and trimer (*m/z* 904) also showed fragmentation pattern that characterizes these compounds.

Conclusion

Direct infusion ESI(-)-MS is a method that provided a quite comprehensive understanding of compounds in *S. obovatum* extracts. SOHE are rich in catechins, flavonoids and flavonols. These compounds in SOHE extracts are related as biological active. For this reason more studies are underway in our lab.

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