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Application of ion mobility-mass spectrometry hyphenated to HPLC in urine studies of flavones metabolites: A real example on the characterization of Diosmine metabolites

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Abstract

Flavonoids are a wide group of molecules present in several foods with important actions in humans. These compounds presents quite similar chemical structures and undergo quite complex metabolization process mainly of phase II with formation of glucuronide, sulfates and mixed conjugates. Their identification and quantitation is very complex because several compounds have identical molecular weights or differentiate by few mass units. In this context also a powerful and selective analytical tool like HPLC-MS/MS may prove inadequate to selectively evaluate flavonoid metabolites.

In recent years ion mobility, coupled with mass spectrometry (IMS-MS and IMS-MS/MS), has become available and unprecedent capabilities, to separate isobaric compounds, are now available. In the present study the results obtained on the caracterization and quantitation of diosmin metabolites by IMS-MS/MS are presented.

As already reported diosmin is absorbed as the aglicone diosmetin and only conjugate metabolites are present in plasma. In urines the main metabolites are glucuronides however the high selectivity of the analytical approach used has permitted to quantify also sulfate and sulfo/glucuronide conjugates presents at very low concentrations without interferences by othe flavonoid conjugates, like the one of hesperetin and quercetin, with just 2 or 4 mass units differences. The sensivity of the analytical method was not compromised being in the pg/ml range.

In conclusion HPLC-IMS-MS/MS has proven to be a very effective tool for the investigation of complex metabolomics problems of natural products adding a new dimension, based on ions conformation, to mass spectrometry.