Identification of bioactive molecules with mass spectrometry

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Bioactive compounds have not been considered as nutrients in food but several important activities in keeping a healthy human body have been attributed to them. Among these bioactive compounds polyphenolics deserve to be mentioned. Flavonoids and phenolic acids are detected in several fruits, vegetables and medicinal plants. Medicinal plants have been used through the ages with the objective of healing different diseases but, only recently in the human history, the reason for some of these attributes were identified and the molecular origin of these effects studied. The reason for studying these medicinal plants has two main goals either to explain the biological effects ascribed to their consumption or to find new molecules that could be used as leads in developing pharmaceutical drugs. Our group has been concerned with the first objective, trying to explain if the herbal infusions could have any real molecular explanation for the ethno-pharmaceutical uses described and if some advantage could be taken from food residues in order to develop functional foods (foods that could have some bioactivity besides their nutritional value). In this context, agricultural residues from pruning of fruit-trees were recently studied with the help of mass spectrometry to identify the compounds present in water extracted leaves. LC-DAD-MS/MS allowed the identification of flavonoids compounds (rutin, quercitrin) and diterpenoids like (O-hexoside triterpenic) in these aqueous extracts. Besides this identification, metabolites of compounds detected in herbal infusions were also identified in the blood and brain of laboratory animals to whom infusion were administered, thus corroborating the bioactivities measured with animal brain enzymes (acetylcholinesterase inhibition). This technique helped the development of metabolomics of phenolic compounds in vivo giving some molecular explanation concerning bioactivities, like enzyme inhibition, cholesterol permeation reduction in cell monolayers found with the laboratory experiments (hypocholesterolemic effect).

Biography
Serralheiro M L M has been involved since last 10 years in the study of herbal infusions composition and their bioactivity in order to explain at molecular level some of the ethno-pharmaceutical applications attributed to them. She has been teaching in the Faculty of Science at University of Lisbon (FCUL), Portugal. She has participated in the Coordination of the Research Center (Centre of Chemistry and Biochemistry) as well as in the Chemistry & Biochemistry Department of FCUL. She has also coordinated several research projects.

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