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Herbal infusion alkaloid profiles by high resolution mass spectrometry

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Herbal infusion products are worldwide consumed for "natural" medical treatments or for maintaining good health. Often these beneficial effects are due to the presence of the alkaloid (alk) compounds contained in the herbs.

Alks are extremely varied groups of organic nitrogen-containing compounds and they have been studied for over 150 years by phytochemists for their physiological action on humans and animals. Usually considered as simple waste products of plant metabolic processes, the highly differentiated chemical structure suggests that they play various specific biological roles. Some alkaloids have toxic effects: pyrrolizidine alks (PA), for example, belong to the most studied group due to increased awareness of its potential risk that prompted the EFSA to publish a specific scientific opinion on PAs in food [EFSA Journal, 2011].

Some studies suggest that commercial preparations for herbal infusions may contain high amounts of alkaloids, in particular of PAs, exceeding the current recommendations.

In this work we present a method that combining the SPE-on line sample pretreatment with the high resolution mass analysis (Q-Orbitrap) allowed the extensive alk characterization of 127 herbal products available as individual "herbs" (dandelion, melissa, dill, etc.) and 7 herbal blends for infusion. The mass spectrometer was operated in positive ion mode and mass spectra were acquired in full MS-data dependent MS/MS analysis at mass resolving power of 140.000.

35 alks were identified and quantified in reference to the pure analytical standards, 48 were confirmed for chromatographic retention time and fragmentation profile analyzing the extracts of herbs already well documented in literature, and other 200 alks were identified using literature information regarding exact mass and isotopic pattern.

Among the 35 target alks, PAs were the most commonly present (26% of samples), with concentrations generally ranging from 0.8 μ g Kg-1 to 2.3 mg Kg-1. The most well-represented was Lycopsamine (13% of samples).

Keywords: herbal infusion, alkaloids, Orbitrap