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Glycoalkaloid profiles of herbal infusion using neutral loss - high resolution mass spectrometry

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Herbal infusions are consumed worldwide thanks to their "natural" beneficial effects; however, they often need specific controls to evaluate the possible presence of alkaloids (alks) [1]. Alks, widespread in nature, are nitrogen-containing organic constituents occur mainly in plants as secondary metabolites. These compounds can arise from amino acid metabolism or from amination of other substrates, which may be, for example, terpenes or steroids [2]. The biosynthesis often involves a further glycosylation of the alks (aglycones) as glycoalkaloids (glyalks) [3]. Alks have long been studied due to their specific toxicological characteristics, as some of them are suspected of having very dangerous properties, although the corresponding glycosylated forms are only rarely considered.

This study aims to investigate the profile of glycoalks belonging to the most important chemical classes (indole, piperidine, protoalkaloid, pyridine, pyrrolidine, pyrrolizidine, quinoline, steroidal, terpenoid, and tropane alks) of a wide selection of commercial herbal tea products (n=120), using a UHPLC equipped with an SPE on-line system and performing the separation on a byphenyl column. The binary mobile phase was composed of 0.1% formic acid (FA) with 5mM ammonium acetate (AAc) and MeOH/ACN 95:5 v/v with 0.1% FA and 5 mM AAc. A Full MS/AIF/NL dd-MS^2 experiment was performed in positive ion mode with the resolution set at 140,000 FWHM (m/z 200; 1.5 Hz) for full MS spectra, at 70,000 FWHM (3 Hz) for AIF and at 17,500 FWHM (12 Hz) for dd-MS^2 [4]. Neutral losses of pentose (m/z 132.0423), deoxyhexose (146.0579), hexose (162.0528), and of all the combinations of up to four of these sugar units were considered.

26 glycoalks were detected, including 9 new glycoalks never before reported in the literature. 28% of samples presented at least one glycalk, being *Escholtzia californiea* the richest one.
This study indicated the presence of the glycosidic forms in several commercial herbal teas used for domestic infusion, permitting higher awareness of the possible risks and benefits relating to the consumption of these products.

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