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BOOK of ABSTRACTS

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926 - GLYCOALKALOIDS IN PLANTS USING HIGH RESOLUTION MASS - NEUTRAL LOSS APPROACH

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Introduction:
Alkaloids (alks) arewidespreadin nature. These nitrogen-containing organic constituentsoccur mainly in plantsas secondary derivatives of the amino acid metabolism, or arising from amination of other substrates, which may be, for example, terpenes or steroids [1]. The biosynthesis often involves a further glycosylation of the alks(aglycones) asglycoalkaloids (glyalks) [2]. One of the best-known glyalks is the steroidal Solanine, a poisonous compound present in the Solanaceae plant family, but, to date, only a few studies on glyalksbelonging to other chemical categories have been reported.

Methods:
The chromatographic separation was performed using a UHPLC equipped with anSPE on-line systemand a byphenyl column. The binary mobile phase was composed of 0.1% formic acid(FA) with 5mM ammoniumacetate (AAc) and MeOH/ACN 95:5 v/v with 0.1% FA and 5 mMAAc. AFull MS/AIF/NL dd-MS2 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-MS2.

Results:
Neutral losses of pentose(m/z 132.0423), deoxyhexose(146.0579), andhexose (162.0528), and of all the combinations of up to four of these sugar units wereconsidered.Full MS and AIF spectra were processed comparing the possible glyalks masses with the corresponding aglycone mass of about 100alksalready reported in literature as characteristic ofthe examined herbs [3,4]. If both the glycoside (in full MS) and the aglycone(in AIF spectra) peaks were present at the same retention time, a manual interpretation of spectrawas performed.The compound identification was assessed consideringthe matching of glycosidicexperimental dd-MS2 spectra with the fragmentation patterns of previously studied alks. The study allowed us to describe theprofilesof glyalksbelonging to the most important chemical classes (indole, piperidine, protoalkaloid, pyridine, pyrrolidine,pyrrolizidine, quinoline, steroidal,terpenoid, and tropanealks) in a selection of 21 plants.

Conclusions
This high resolution mass/neutral loss experiment permitted us to describe the presence of the glycosidic forms of a large selection of alks, permittinghigherawareness of the possible risks and benefits relating to the consumption of popular plant-based medicines with new attention to both the free and bond alk forms.

Novel Aspect:
To our knowledge, this is the first high-resolution mass - neutral loss approach proposed for a broad identification of plantglyalksbelonging to the main chemical classes.

References
Aniszewski T., Alkaloid Chemistry, Biological Significance, Application and Ecological role, 7-10 (2007).
Itkin M., Rogachev I., Alkan N., Rosenberg T., Malitsky S., Masini L., Meir S., Iijima Y., Aoki K., de Vos R., Prusky D., Burdman S., Beekwilder J., Aharoni A., The Plant Cell, 23, 4507-4525 (2011).
Nardin T., Piasentier E., Barnaba C., Larcher R., J Mass Spectrom, 51, 729-741 (2016).
Nardin T., Piasentier E., Barnaba C., Larcher R., Drug Test Anal, 10, 423-448 (2017).