



XXV RNE - IX CIE ESPECTROSCOPIA

**XXV NATIONAL SPECTROSCOPY
MEETING (XXV RNE)**

**IX IBERIAN SPECTROSCOPY
CONFERENCE (IX CIE)**

Alicante, 20th-22nd July 2016

Book of abstracts

Determination of atropine and scopolamine in buckwheat and related products using modified QuEChERS and liquid chromatography tandem mass spectrometry

J. Marín-Sáez^{1,*}, H. Chen^{1,2}, R. Romero-González¹, R. López-Ruiz, A. Garrido-Frenich¹.

¹University of Almería, Department of Chemistry and Physics, Research Centre for Agricultural and Food Biotechnology (BITAL), Agrifood Campus of International Excellence ceiA3, Carretera de Sacramento s/n, E-04120 Almería, Spain.

²Chinese Academy of Agricultural Sciences (TRICAAS), Tea Research Institute, 9 South Meiling Road, 310008, Hangzhou, China.

*jms485@inlumine.ual.es

Buckwheat is a healthy pseudo cereal widely cultivated over the world as an important raw material used for functional food because it becomes a dietary source of bioactive compounds, such as nutritionally valuable protein, phenolic compounds, starch and dietary fiber, essential minerals and trace elements. However, buckwheat can be contaminated by stramonium (*Datura stramonium*), which can contain high concentration of tropane alkaloids, and therefore, these toxic substances can be found in buckwheat and related matrices at concentrations higher than 100 µg/kg [1].

Tropane alkaloids are synthesized by the plants of the genus from *Solanaceae* family, although they are also produced in smaller quantities in plants from other families. They can affect human and animal health due to their high toxicity and intake of contaminated food or animal feed. Although there are more than 200 tropane alkaloids, atropine and scopolamine are the most common compounds of this family.

According to the EFSA scientific opinion in 2013 [1] more attention must be focused on the contaminated levels of atropine and scopolamine in food from plant origin, such as cereal products, grain-based baby-food, buckwheat grain and food products and tea and herbal infusions. Therefore, the development of quick, easy and reliable analytical methods for the trace analysis of tropane alkaloids at trace levels in food from plant origin is desirable.

Therefore the aim of this study is the development and validation of an analytical method for the simultaneous determination of atropine and scopolamine residues in buckwheat and related products. A modified QuEChERS (Quick, Easy, Cheap, Effective, Rugged and Safe) extraction method with acidified acetonitrile (1% formic acid v/v) followed by a clean-up step using graphitized black carbon (GBC) and primary secondary amine (PSA) was applied. For the separation and quantification of the target compounds, ultra high performance liquid chromatography (UHPLC)-coupled to tandem mass spectrometry (MS/MS), utilizing triple quadrupole (QqQ) as analyzer, was used. The method was validated, determining linearity, trueness, precision, limits of detection (LODs) and quantification (LOQs). Recoveries ranged from 75 to 92% with precision below 17% (RSD values) for all the compounds studied. Both LODs and LOQs were below 2 µg kg⁻¹.

The validated method was tested in eight commercial samples (buckwheat, wheat, soy, buckwheat flour, buckwheat noodle, amaranth grain, chia seeds and peeled millet). Target compounds were not found above the detection limits of the method.

Acknowledgements

The authors gratefully acknowledge the Spanish Ministry of Economy and Competitiveness (MINECO) and FEDER (project ref. CTQ2015-69899-R).

References

[1] EFSA. Scientific opinion on tropane alkaloids in food and feed, EFSA panel on contaminants in the food chain (CONTAM). *The EFSA Journal*, **11**, 3386-3499 (2013).