

P42

Metabolomic fingerprinting/profiling employing DART-OrbitrapMS and UPLC-ESI-OrbitrapMS for DDGS authenticity and traceability

H. Novotna, T. Cajka, M. Tomaniova, J.Hajslova

Institute of Chemical Technology, Prague, Department of Food Analysis and Nutrition, Technicka 3, 166 28 Prague 6, Czech Republic

E-mail: Jana.Hajslova@vscht.cz

Abstract Distillers dried grains with solubles (DDGS) are the by-products from bio-ethanol production. In this study, the methods based on metabolomic fingerprinting/profiling for authenticity and traceability of samples originating from different countries (USA, China, Germany) were evaluated. For the extraction, a methanol/water mixture and cyclohexane were chosen as the best solvents to obtain a broad spectrum of metabolites.

Instrumental analyses were performed using ambient mass spectrometry [Direct Analysis in Real Time (DART) ion source] and liquid chromatography with electrospray (LC-ESI), both coupled with a high-resolution Orbitrap mass spectrometer. Also, identification of some markers has been conducted. In an organic fraction, triacylglycerols were the main group of identified analytes, while in an aqueous fraction, mainly organic acids, amino acids and sugars were found. Samples were classified using sophisticated chemometric tools.



Keywords metabolomic;fingerprinting/profiling;DDGS;DART-OrbitrapMS;UHPLC-OrbitrapMS;authenticity;traceability;chemometrics

Acknowledgement The research leading to these results has received funding from the European Community's Seventh Framework Programme (FP7/2007-2013) under grant agreement n° KBBE-265702 (QSAFFE)

This communication is under the responsibility of the authors and does not reflect the view of the European Union Commission.