



11th International Symposium on RECENT ADVANCES IN FOOD ANALYSIS

November 5-8, 2024 • Prague, Czech Republic



Vibrational spectroscopy and chemometrics workshop

Tuesday, 5th November 2024, 9:00 - 13:00

Chaired by:

Vincent Baeten (v.baeten@cra.wallonie.be)

François Stevens (f.stevens@cra.wallonie.be)

Walloon Agricultural Research Center (CRA-W)

Quality and authentication of agricultural products Unit

Gembloux, Belgium

TUESDAY, November 5, 2024

9:00-13:00

WORKSHOP on Vibrational spectroscopy and chemometrics

Moderators:

Vincent Baeten & François Stevens

Walloon Agricultural Research Centre (CRA-W), Gembloux, Belgium



8:30-9:00		Registration & Welcome Coffee
9:00-10:00	W1	BASICS OF VIBRATIONAL SPECTROSCOPY <i>Vincent Baeten, Walloon Agricultural Research Centre, Belgium</i>
10:00-11:00	W2	BASICS OF CHEMOMETRICS <i>François Stevens & Juan A. Fernández Pierna, Walloon Agricultural Research Centre, Belgium</i>
11:00-11:30		Coffee break
11:30-11:55	W3	COMPARATIVE ANALYSIS OF SPECTROSCOPIC TECHNIQUES FOR ENHANCING HAZELNUT VARIETAL AND GEOGRAPHICAL AUTHENTICATION <i>Berta Torres Cobos, University of Barcelona, Spain</i>
11:55-12:20	W4	STRESS DETECTION/ASSESSMENT IN DAIRY COWS BY THE DETERMINATION OF CORTISOL IN HAIRS BY NEAR-INFRARED (NIR), MID-INFRARED (MIR) AND RAMAN SPECTROSCOPY <i>Octave Christophe, Walloon Agricultural Research Centre, Belgium</i>
12:20-12:45		Last remarks <i>Vincent Baeten, Walloon Agricultural Research Centre, Belgium</i>
12:45-13:00		Discussion & Conclusions

Introduction

Vibrational spectroscopy, as Near infrared (NIR) or Raman, is the most widely used non-destructive technology in the food and feed industries for the daily determination and quantification of qualitative parameters of the materials. The high throughput of the method, the capacity to determine in one single analysis a panoply of parameters, the possibility to build a network of spectrometers together with its potential use both on-line and at-line in a production plant made this technique even more attractive. These techniques provide real-time analyses with an increased sample throughput. Moreover, more recent areas as hyperspectral imaging allow collection of spectroscopic images at different levels from single kernel or particle levels to satellite. This is of great interest for laboratories that control feed compound or cereals. Other decisive advantages of spectroscopic methods are the ability to determine simultaneously different parameters and criteria, no use of reagents and reduced sample preparation.

The combination of these techniques with appropriate data treatment or chemometric tools should help to solve the deep and rapid changes that the agro-food sector is facing with increasing consumer concerns about food and feed safety and quality issues. These concerns arise in part from previous safety crises (e.g. dioxin, BSE, melamine) and in part from the health impact of food and feed. The main outcome of these consumer demands is an increased need for appropriate techniques and methods to help producers, retailers and processors to control and to track their products. Infrared and Raman spectroscopy combined with chemometric should allow to build strategies that can be applied to check (on-line, at-line and at the laboratory level) the quality of food and feed materials, to detect non conformity and subsequently to identify targeted or untargeted adulterants and contaminants among others.

Speakers



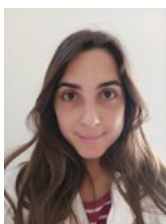
Dr. Ir. Vincent BAETEN got his Engineer degree in Agronomy (1993) and PhD (1998) in Agricultural Sciences from the Catholic University of Louvain (Belgium). He has been awarded of a Marie-Curie Fellowship (1996-1998) at the Instituto de la Grasa of the CSIC (Spain). He is head of the Food and Feed Quality Unit of the Valorisation of Agricultural Products Department of Agricultural products of Walloon Agricultural Research Centre (CRA-W, Gembloux - Belgium). The Food and Feed Quality Unit is involved in the development of rapid, multi-analytes and untarget methods based on electronic and vibrational spectroscopy (Fluorescence, VIS, NIR, NIR imaging, MIR, Raman), optical microscopy and chemometrics. Vincent Baeten is deputy director of the European Union Reference Laboratory for Animal proteins in feedingstuffs (EURL-AP, <http://eurlap.craw.eu>). Since 2013, he is also invited professor at the Catholic University of Louvain (UCL). He has been awarded of the 2011-Q-Interline Sampling Awards for the outstanding contribution in sampling applied to spectroscopy methods. He has published more than 110 scientific papers and book chapters.



Dr Juan Antonio FERNANDEZ PIERNA got his Degree in physical chemistry at the University of Zaragoza, Spain in 1997. Afterwards, in 2003, he obtained his PhD in Pharmaceutical Sciences (Chemometrics) at the Analytical Chemistry department of the Vrije Universiteit Brussel (Professor D. L. Massart) with a thesis entitled "Improvements in the multivariate calibration processes". Since 2003 he works as research assistant at the CRA-W in Belgium where he has been working for the statistical treatment of the data, the application of chemometrics and the validation of methods. From end 2009, he is also responsible of the Hyperspectral Imaging laboratory installed at the Food and Feed Quality Unit. He is author or co-author of 9 book chapters and around 65 scientific papers mainly related to the statistical treatment of spectroscopic data (including homogeneity detection and uncertainty estimation), food and feed authentication and imaging techniques. He is a member of the Belgian Chemometric Society and he was and is still involved at different EU projects: STRATFEED, TYPIC, TRACE, FEED SAFETY, SAFEED-PAP, QSAFFE, FOODINTEGRITY.



Dr François STEVENS got a Degree in Physics with specialization in spectroscopy from the Université Libre de Bruxelles and a Phd in Agricultural Sciences (spatial statistics for soil science) from the Université catholique de Louvain. He has also made applied research on solar radiation at the Royal Belgian Institute for Space Aeronomy. Since 2019 he works as research assistant at the CRA-W. He deals with visible and NIR spectral data and hyperspectral images for different applications such as detection of constituents in food, agricultural or industrial products and plant disease monitoring. He has a strong expertise in statistical modelling, machine learning and data visualization.



MSc Berta TORRES obtained her Degree in Chemistry in 2018 and Master in Analytical Chemistry in 2019 from the University of Barcelona (Spain). She currently works as a research assistant in the "Lipids and Bioactive Compounds in the Food Chain" (LiBiFOOD) group at the same university. Her research focuses on developing analytical tools to authenticate the varietal and geographical origin of food products that are highly susceptible to fraud. She is also in the final stages of completing her doctoral thesis on this subject.

MSc Octave CHRISTOPHE completed his analytical chemistry degree at the University of Namur, Belgium, in 2018. He has been working at the Walloon Agricultural Research Centre in Belgium since 2019, focusing on analytical research in the dairy sector. His role involves a diverse array of tasks, including spectroscopy, spectral standardization, chromatography, and chemometrics. His research is centered on milk spectra, specifically in the development of prediction equations for fatty acids and free fatty acids, as well as contributing to the improvement of the European spectral standardization network. Since 2022, he has also been pursuing a PhD thesis in collaboration with the University of Liège, under the guidance of Prof. Soyeurt and Dr. Baeten, concentrating on the development of prediction equations for free fatty acids using various machine learning algorithms.