Cover story

Volatile compounds profiling by using proton transfer reaction-time of flight-mass spectrometry (PTR-ToF-MS). The case study of dark chocolates organoleptic differences
By Zoé Deuscher, Isabelle Andriot, Etienne Sémon, Marie Repoux, Sébastien Preys, Jean-Michel Roger, Renaud Boulanger, Hélène Labouré and Jean-Luc Le Quéré

Pages 92–119

The full featured article is available at http://onlinelibrary.wiley.com/doi/10.1002/jms.4317/pdf
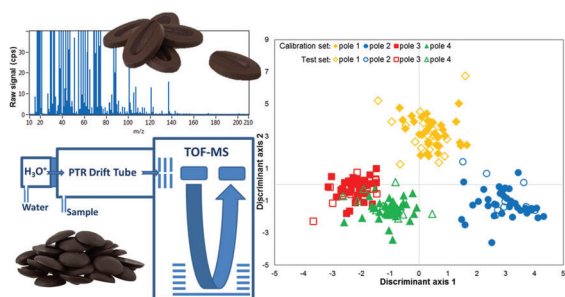
Ahhhh chocolate! Who doesn't love chocolate? The analysis of volatile organic compounds (VOCs) emanating from environment, plants, food or food ingredients has been the basis for many studies aiming at categorizing samples or sites. For this purpose, global VOCs profiles may be used as fingerprints of the samples, sometimes referred to as "volatilome". In this special feature, Jean-Luc Le Quéré and co-workers use proton transfer reaction mass spectrometry (PTR-MS) coupled to a time-of-flight (TOF) mass analyzer to classify over 200 dark chocolate samples based on their content in VOCs. The final goal was to build a model based on the PTR-MS monitored dark chocolates volatilome that could be used to predict the four distinct sensory poles previously defined based on the flavor of cocoa from diverse origins and cultivars. Jean-Luc Le Quéré is a Senior Researcher at the Center for Taste and Feeding Behaviour of the Institut de Recherche Agronomique (INRA) of Bourgogne-Franche-Comté (France). The general objective of this center is to get a better understanding of the physicochemical, molecular, cellular, behavioral and psychological mechanisms underlying sensory perception of food, eating behavior and health consequences.

Authors' biographies

Zoé Deuscher graduated with an MSc in Plant Biology from the University of Strasbourg. She is currently in her last year of her PhD thesis at INRA Dijon, Centre des Sciences du Goût et de l'Alimentation (CSGA), on differentiation of dark chocolates varying in sensory characteristics using analytical chemistry tools (GC-O-MS, PTR-MS).

Isabelle Andriot graduated with an MSc in Chemistry from the University of Burgundy in Dijon. Since 1998, she has been working at INRA, Dijon, where she develops tools for studying aroma release in foods and their characterization using PTR-MS within the ChemoSens Platform of CSGA.

Etienne Sémon is an engineer in analytical chemistry. He earned his diploma from the Conservatoire National des Arts et Métiers (CNAM). He is a specialist in analysis and identification of volatile compounds by GC, GC-MS and GC-FTIR. For more than fifteen years he has devoted his work within the ChemoSens Platform of CSGA on *in-vitro* and *in-vivo* flavour release using soft ionization mass spectrometry such as APCI-MS and PTR-MS.

Marie Repoux earned a degree in Food Science Engineering in 2007 and a PhD in Food Science in 2012 from the University of Burgundy in Dijon focused on *in-vivo* aroma release. She has been working at Valrhona since 2011, first as Sensorial Analysis Manager and currently as Business Analyst.

Sébastien Preys graduated with an MSc in Food Science and earned a PhD degree in Analytical Chemistry and Chemometrics. He has been working for 12 years at Ondalys, a French company providing expertise, services and trainings for Chemometrics, Machine Learning and Data Mining.

Jean-Michel Roger is a researcher in chemometrics, mainly applied to the development of sensors for agriculture and the environment. As part of the IRSTEA COMiC team, he is studying the robustness of calibration models related to near-infrared spectrometry. In this context, he has developed methods for selecting spectral characteristics and in particular for selecting variables. He is also involved in worldwide development of chemometrics, participating in the organization of conferences and structuration of networks, nationally and internationally.

Renaud Boulanger, PhD, is the head of the team "Sensory quality of fresh and processed products" in the Joint Research Unit "Qualisud" in CIRAD, Montpellier. His first research topic is on biochemistry of secondary metabolites, particularly on aroma formation in relation with genetic, technological and environmental factors on tropical products like coffee, rice, fruit and especially cocoa. His second research interest is on the development of fingerprint techniques for the characterization of quality attributes and discrimination of food products.

Hélène Labouré earned a PhD in Food Science from the University of Burgundy in Dijon. She is an Assistant Professor at AgroSup Dijon, an engineer school in agronomy and agri-food. She performs her research at CSGA where she works on the relationship between aroma release and aroma perception. Her research takes into account food properties (particularly texture) but also oral physiology of the subjects.

Jean-Luc Le Quéré is a senior scientist in the Flavour, Food Oral Processing and Perception research group of CSGA, INRA Dijon. He earned a PhD degree in Chemistry from the University of Western Brittany in Brest in 1982 and the habilitation degree in Chemistry from the University of Burgundy in Dijon in 1995. After a post-doctoral stay at the University of Glasgow (UK) in the Department of Chemistry, he joined the Aroma Research Laboratory of INRA in Dijon as an analytical chemist in 1983. At CSGA he is now in charge of methods development dealing with *in-vitro and in-vivo* flavour release using atmospheric pressure chemical ionization mass spectrometry (APCI-MS) and proton transfer reaction mass spectrometry (PTR-MS).