



# Nose-space of dark chocolates using PTR-ToF-MS and link to flavour perception through simultaneous Temporal Dominance of Sensations (TDS)

Zoé Deuscher, Isabelle Andriot, Sylvie Cordelle, Marie Repoux, Renaud Boulanger, Hélène Labouré, Pascal Schlich, Jean-Luc Le Quéré

## ► To cite this version:

Zoé Deuscher, Isabelle Andriot, Sylvie Cordelle, Marie Repoux, Renaud Boulanger, et al.. Nose-space of dark chocolates using PTR-ToF-MS and link to flavour perception through simultaneous Temporal Dominance of Sensations (TDS). .22. International Mass Spectrometry Conference (IMSC 2018), Aug 2018, Florence, Italy. hal-02931982

**HAL Id: hal-02931982**

**<https://hal.inrae.fr/hal-02931982>**

Submitted on 7 Sep 2020

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.



Società Chimica Italiana  
Divisione di Spettrometria  
di Massa



# XXII International Mass Spectrometry Conference

Florence (Italy) - August 26-31, 2018



# ABSTRACT BOOK



Società Chimica Italiana  
*Divisione di Spettrometria  
di Massa*



# XXII International Mass Spectrometry Conference

# ABSTRACT BOOK

Florence (Italy) – August 26-31, 2018

---

## TABLE OF CONTENTS

---

<i>IMSF Executive Committee, IMSF National Affiliates</i> .....	4
<i>IMSC 2018 Scientific Committee</i> .....	5
<i>Oral communications</i> .....	6
a. <i>Sunday, August 26</i> .....	7
b. <i>Monday, August 27</i> .....	8
c. <i>Tuesday, August 28</i> .....	61
d. <i>Wednesday, August 29</i> .....	114
e. <i>Thursday, August 30</i> .....	164
f. <i>Friday, August 31</i> .....	214
<i>Poster communications</i> .....	240
a. <i>Monday, August 27</i> .....	241
b. <i>Tuesday, August 28</i> .....	510
c. <i>Wednesday, August 29</i> .....	775
d. <i>Thursday, August 30</i> .....	1019
<i>Author Index</i> .....	1246

# XXII International Mass Spectrometry Conference

MOr.05-3

## **NOSE-SPACE OF DARK CHOCOLATES USING PTR-TOF-MS AND LINK TO FLAVOUR PERCEPTION THROUGH SIMULTANEOUS TEMPORAL DOMINANCE OF SENSATIONS (TDS)**

**Zoé Deuscher** <sup>(1)</sup> - **Isabelle Andriot** <sup>(1)</sup> - **Sylvie Cordelle** <sup>(2)</sup> - **Marie Repoux** <sup>(3)</sup> - **Renaud Boulanger** <sup>(4)</sup> - **Hélène Labouré** <sup>(5)</sup> - **Pascal Schlich** <sup>(1)</sup> - **Jean-Luc Le Quéré** <sup>(6)</sup>

<sup>(1)</sup> INRA, CSGA, Dijon - <sup>(2)</sup> CNRS, CSGA, Dijon - <sup>(3)</sup> Valrhona, Valrhona, Tain-l'Hermitage - <sup>(4)</sup> CIRAD, Qualisud, Montpellier - <sup>(5)</sup> AgroSup Dijon, CSGA, Dijon - <sup>(6)</sup> INRA, Centre des Sciences du Goût et de l'Alimentation (CSGA), Dijon

**Keywords:** chocolate – nosespace – PTR-ToF-MS – Temporal Dominance of Sensations (TDS)

### **Introduction**

Aroma of dark chocolate depends on process and cocoa origin and variety. A sensory analysis of 206 standardized chocolates produced from various cocoa beans classified them in four sensory categories. These categories were confirmed in a PTR-MS analysis of the chocolates volatilome [1]. The objective here was to study the nosespace of a subset of chocolates simultaneously with their temporal profile to better explain the sensory categorization at a perception level.

### **Methods**

A Temporal Dominance of Sensations (TDS) evaluation of 8 chocolates (2 selected per category) was done in triplicate by 12 subjects while the aroma released in their nose were simultaneously collected and injected into a PTR-ToF-MS. The two sets of data were analyzed conjointly by defining an index of abundance of each detected aroma compound while a given attribute was dominant: the Abundance While Dominance (AWD) index [2].

### **Results**

TDS is able to dynamically capture multidimensionality of perception. The obtained TDS curves clearly differentiated the chocolates that were regrouped by sensory category as revealed by a principal component analysis (PCA). The dynamics of perception have been considered only scarcely in comparison to simultaneous in vivo aroma release over time measured by on-line mass spectrometry (nosespace). Computation of the AWD indices at individual level allowed to statistically assess the differences between the products over subjects and replicates and assessed statistically the relationships between the two sets of data. Through correspondence analyses (CA) some relationships between certain aroma compounds and the sensory attributes expected to be related to them were found. Although in previous studies pairing nosespace and TDS various temporal links could be proposed [3], no clear relationships could be safely established due to the fact that the conclusions were mainly based on a descriptive analysis of the data conducted at panel level.

### **Conclusions**

Pairing nosespace with Temporal Dominance of Sensations evaluation of dark chocolates categorized in four sensory groups provides meaningful data that can be analyzed at individual level thanks to the AWD indices. Descriptive multivariate analyses of these AWD indices gave interesting clues on the relationships between the aroma compounds released in mouth and their expected perceived sensory attributes.

### **Novel Aspect**

Pairing nosespace PTR-ToF-MS with Temporal Dominance of Sensations allows assessing the relationships between aroma compounds released in vivo and their perception.

### **References**

1. Deuscher Z., Andriot I., Sémon E., ..., Le Quéré J.L., *SMMAP2017*, Dineyland Paris, October 2-5 (2017).
2. Schlich P., Thomas A., Visalli M., Labarre D., Sémon E., Le Quéré J.L., in *Flavour Science: Proceedings of the XIV Weurman Flavour Research Symposium*, (Taylor A.J., Mottram D.S., Eds.), Context Products Ltd., Leicestershire (UK), 327-332 (2015).
3. Déléris I., Saint-Eve A., Dakowski F., Sémon E., Le Quéré J.L., Guillemin H., Souchon I., *Food Chem.*, 127(4), 1615-1624 (2011).