



Società Chimica Italiana  
Divisione di Spettrometria  
di Massa



FONDAZIONE  
EDMUND  
MACH ■■■

# **3<sup>rd</sup> MS-Wine Day**

**May 16 - 17, 2019**



**Fondazione E. Mach**  
**San Michele all'Adige (Trento)**

**Mass Spectrometry & Grapes, Wines, Spirits**

**CONFERENCE PROCEEDINGS**

SESSION 2  
(chairman: Riccardo Flamini)

- 4:50 p.m. Invited speaker **Eduardo Dellacassa** (Universidad de la República de Uruguay)  
"The aroma profiles of South-American wines"
- 5:20 p.m. **Alberto Onzo** (Università degli Studi della Basilicata)  
"Phytochemical screening of new italian wine varieties by using high resolution mass spectrometry"
- 5:35 p.m. **Luca Cappellin** (Università degli Studi di Padova / Tofwerk AG, Switzerland)  
"Real-time screening of single corks for TCA and TBA contamination by Vocus CI-TOF"
- 5:50 p.m. **Alice Sosic** (Università degli Studi di Padova)  
"Polyphenols derived from wine aged in oak barrels inhibit HIV-1 nucleocapsid protein"
- 5:55 p.m. **Christine Mayr Marangon** (Institute for the Dynamics of Environmental Processes-CNR, Venice)  
"GC/MS characterization of the aromatic profile of wines made from resistant varieties and mountain cheeses from the Belluno area"
- 6:00 p.m. **Iuliia Khomenko** (Fondazione Edmund Mach, San Michele all'Adige)  
"Improved understanding of flavor generation in beer through the use of proton transfer reaction time of flight mass spectrometry"
- 6:05 p.m. **Nicola Cimino** (Agilent Technologies)  
"Migliori flussi di lavoro per l'autenticità degli alimenti: LC-QTOF 6546 e software suite dedicate"
- 6:20 p.m. Discussion
- 6:40 p.m. End of session
- 6:50 p.m. **Transfer to LaVis winery (10 minutes by car from F. E. Mach)**
- 7:10 - 10:00 p.m. **Guided tour of the winery, complimentary tastings and dinner.**

Friday, May 17, 2019

SESSION 3  
(chairman: Giorgio Nicolini)

- 9:00 a.m. Invited speaker  
**Bruno Fedrizzi** (University of Auckland, New Zealand)  
"Sulfur compounds in wine"
- 9:30 a.m. **Davide Slaghenaufi** (University of Verona)  
"Study of norisoprenoids and terpenes related to tobacco and balsamic notes of Valpolicella wines, the effect of aging"
- 9:45 a.m. **Matteo Perini** (Fondazione Edmund Mach, San Michele all'Adige)  
" $\delta^{15}\text{N}$  and  $\delta^{13}\text{C}$  analyses of amino acids of grape"

## Improved understanding of flavor generation in beer through the use of proton transfer reaction time of flight mass spectrometry

Richter T.<sup>1</sup>, Silcock P.<sup>1</sup>, Eyres G. T.<sup>1</sup>, Khomenko I.<sup>2</sup>, Algarra A.<sup>2</sup>, Bremer P.J.<sup>1</sup>, Capozzi V.<sup>3</sup>, Biasioli F.<sup>2</sup>

<sup>1</sup> Department of Food Science, University of Otago, Dunedin, New Zealand [pat.silcock@otago.ac.nz](mailto:pat.silcock@otago.ac.nz)

<sup>2</sup> Department of Food Quality and Nutrition, Fondazione Edmund Mach, San Michele All'Adige, Italy

<sup>3</sup> Department of the Sciences of Agriculture, Food and Environment, University of Foggia, Foggia, Italy

As the brewing industry looks to create beers with greater flavor diversity, harnessing yeast biotransformations may provide a pathway to achieve this goal. Unfortunately, these pathways for some compounds are still poorly understood. Due to sample preparation and analysis time, gas chromatography techniques are not well suited to monitoring changes in rapidly fermenting systems especially when needing to compare multiple variables simultaneously. Proton transfer reaction time of flight mass spectrometry (PTR-ToF-MS) coupled to an autosampler to provide online measurements during fermentation may provide a pathway to help unlock these pathways.

Two studies were carried out. Study 1 used 2 yeast strains (Scottish ale and California Ale) x 2 hop varieties (Motueka and Nelson Sauvin). Study 2 involved 6 yeast strains (Fermentis WB-06, US-05, S-33, S-189, S-23, and W-34/70) x 1 hop variety (Motueka) studies to help our understanding of how beer flavour is generated and in particular how yeast modulates hop aroma compounds. Both studies used malt extract (120g/L), Waimea bittering hops (0.24 g/L, 20 International bittering units) and aroma hops (5g/L) added for 5 min after 30 min boiling when wort temperature cooled to 90°C.

Using PTR-ToF-MS coupled to an autosampler allowed insights into the release kinetics of volatiles important in beer flavor and allowed multiple variables to be simultaneously examined and replicated. By sampling under dynamic conditions, it was possible for the time of volatile generation to be observed during fermentation. It was found that the magnitude and kinetics of biotransformations are heavily yeast-strain dependent and to adequately describe the formation of these compounds yeast strain variability needs to be considered in experimental designs.