VALORISATION OF PREMIUM ITALIAN WINES BY VOLATILE SIGNATURE EXPLORATION WITH GC×GC-(TOF)MS AND COMPUTER VISION

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INTRODUCTION

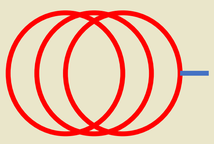
- Computer vision is a branch of artificial intelligence (AI) that allows systems to extract useful information from digital images and make predictions based on that information
- The approach entails creating a cumulative class-image[1] from the combination of chromatographic data from various samples. The pixels (spectral events) from many 2D images are realigned, registered[2], and arithmetically summed to create a cumulative pattern resembling the compositional complexity of all samples within a group

OBJECTIVES

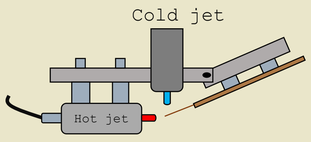
- Examine the volatilome and aroma peculiarities of experimental micro-vinification of Amarone DOCG wine carried out with *Corvina* and *Corvinone* cultivars harvested in different areas.
- Define an automated workflow based on Computer Vision capable to collect the peculiarities of multiple samples belonging to the same class by combining patterns and visually comparing them with the ones of a different class. Once differences are computed, link the pixels to chemical species to explain biological differences

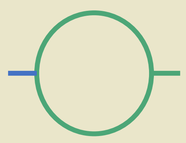
EXPERIMENTAL SETUP AND DATA PROCESSING STEPS

Headspace Solid Phase Microextraction sampling:
(DVB/CAR/PDMS) df 50/30 µm - 2 cm - Supelco (Bellefonte, PA, USA). Wine volume 2.0 mL + deionized water 2.0 mL + 0.500 g sodium chloride (baked in oven prior analysis). Sampling time: 60 min at 40°C under constant stirring



[1]D – Polar (DB-Wax)
30 m × 0.25 mm × 0.25µm
He carrier @ **1.6 mL/min**





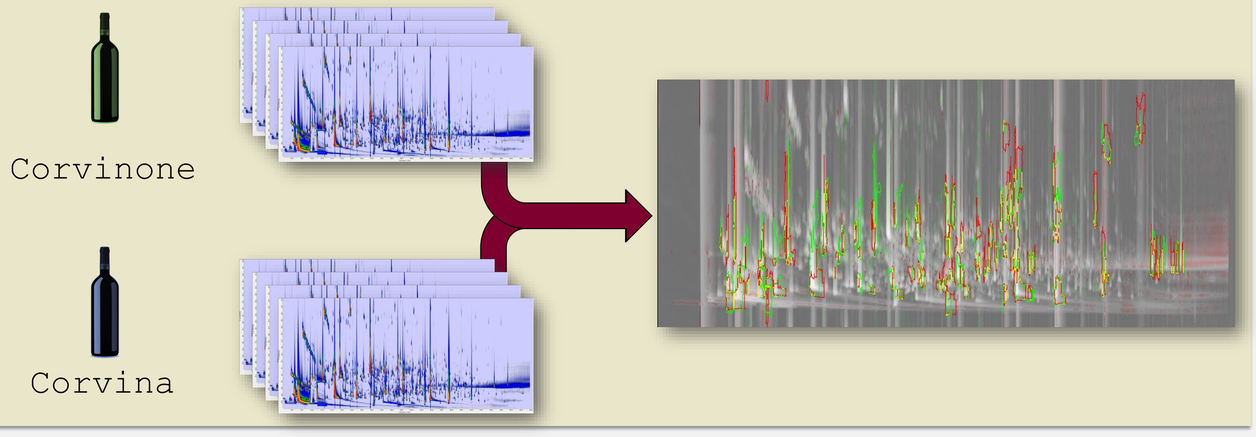
[2]D – Medium polarity OV1701
1.0 m × 0.10 mm × 0.10 µm
He carrier @ **1.6 mL/min**

Mass spectrometry (TOFMS):
Single ionization (70eV)
Source temperature: 290°C
Transfer line: 270 °C
Mass range: 45-600 m/z
Acquisition mode: full scan
Acquisition speed: 100 Hz

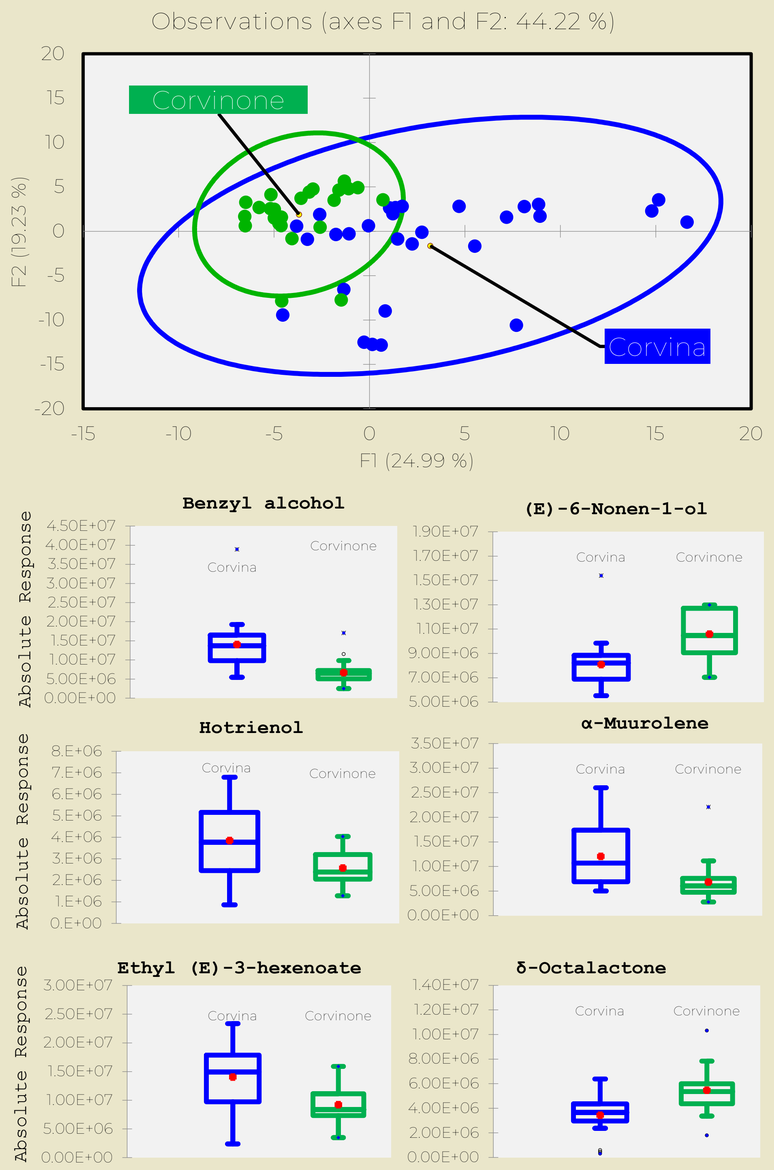
S/SL injector: 280°C, split mode, split ratio 1:20
Oven ramp: 50 °C (2') to 260 °C @ 3.5 °C/min
P_M: 3.5s, hot-jet pulse 250 ms cold jet stream MFC from 40% to 5% in 60 min

Reliable template construction and composite image comparison (GC Image™ & Image Investigator™) - GC Image v2021r2

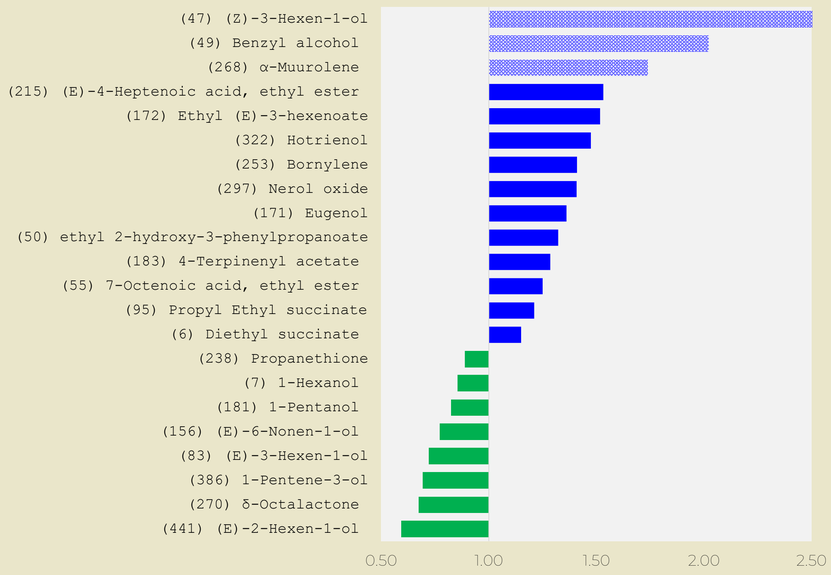
- Data preprocessing (Data import, rasterization, Baseline correction, 2D peaks detection and integration)
- Build a reliable template of known and unknown peaks and peak regions features with image registration and realignment through the use of reliable peaks
- Arithmetically combine class images to create the composite one for each class. Differences on each pixel of the composite images are computed and univocally linked to corresponding peaks through their metadata (1 & 2 I^T, MS spectrum)



RESULTS



The explorative PCA on absolute responses (54 samples x 121 peak regions) suggest that the cultivar dominates sample clustering.
PLS-DA was conducted to select most discriminant variables (42 analytes – 13 tentatively identified). The absolute response of 6 of them are illustrated in the boxplot.
Pairwise comparison between samples through the computer vision approach identified 22 analytes with meaningful variations, that are visualized as fold-change in the bar plot. Bars with shadowed colour are for analytes with RSD%>30



CONCLUSIONS

GC×GC-TOFMS with thermal modulator showed to be a suitable technique to capture the meaningful variations between different wine cultivars harvested in the same geographical region; Alcohols such as 2-Hexenol are predominant in Corvinone cultivar, characteristic of more fruity notes, while terpenes and esters are more abundant in the Corvina, donating herbal flavours.

Computer vision, here exploited for the creation of cumulative images capable to capture all the compositional complexity of all samples within a class and the comparison between them showed to be an interesting approach that is complementary to UT (Untargeted-Targeted) fingerprinting

[1]F. Stilo *et al.*, Food Chem. 340 (2021). DOI: 10.1016/j.foodchem.2020.128135
[2]S.E. Reichenbach *et al.*, J. Chromatogr. A. 1226 (2012). DOI:10.1016/j.chroma.2011.07.046.

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