# Detection of some wine flaws with rapid correlative analytical methods – preliminary results

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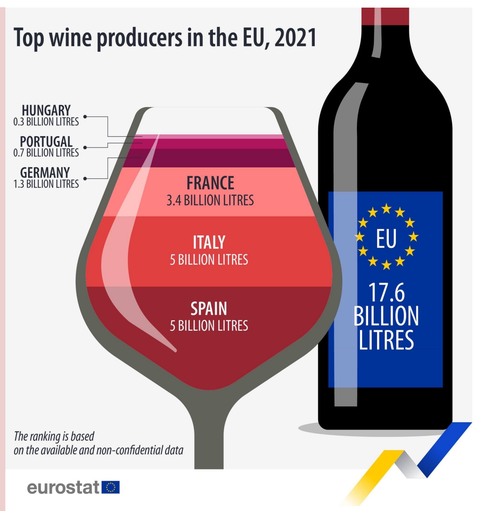
## INTRODUCTION

- Economic relevance of wine production.
- Increasing world-wide demand for high-quality wines → need for instrumental analytical methods to test and monitor the quality in large quantities.
- The correlative analytical technologies offer alternative solutions of the traditional human sensory tests and classical analytical approaches → rapid and accurate quality testing → opportunity for early detection of the appearance of some defects causing wine faults and flaws.

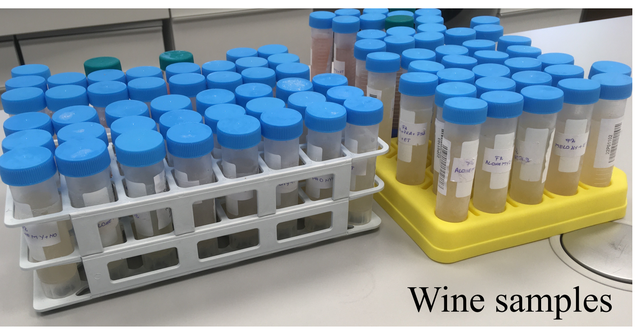



## AIM OF THE STUDY

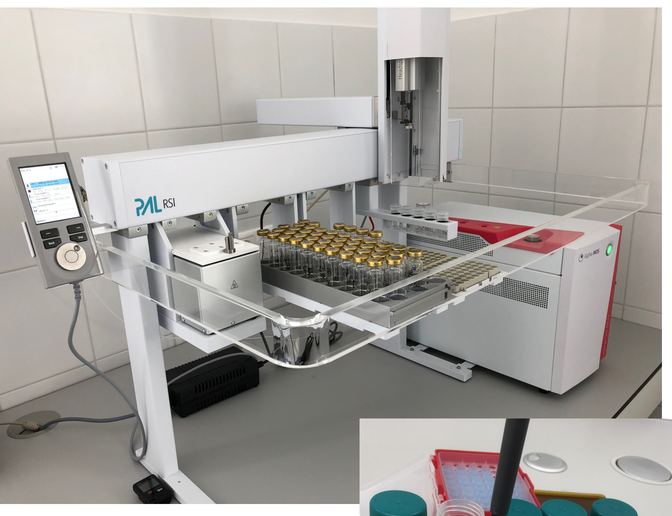
- **Developing testing methods with near-infrared spectroscopy and electronic nose for the rapid detection of wines with artificially caused flaws.**

## MATERIALS AND METHODS

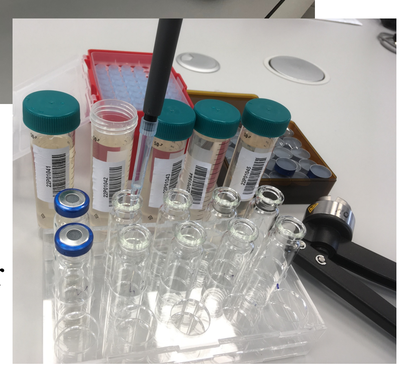
- ***Wines*:** red and white wines with added chemicals
  - Acetic acid (AA) → volatile acidity
  - 4-ethylphenol (4EP) → barn smell (brett wine caused by
  - 4-ethylguaiacol (4EG) → *Brettanomyces* yeasts)
- ***Model solutions*:** water + ethanol + flaw chemicals (AA, 4EP, 4EG) in 0.2, 0.4, 0.8, 2, 4, and 8 mg/L concentrations
- ***Sample preparation*:** adding water, NaCl, $H_3PO_4$ to decrease solubility of gases
- ***Near-infrared spectroscopy (NIRS)*:** Metrohm NIRSystems XDS, transmission mode, 1 mm quartz cuvette, sample temperature: 25 °C
- ***Electronic nose (EN)*:** Alpha MOS Heracles Neo electronic nose with flash GC technology (column #1: MXT-5; column #2: MXT-1701) and PAL autosampler, sample volume 5 ml in 20 ml headspace vials, incubation at 50 °C for 5 min, injected volume 1 ml, trap temperature 40 °C, carrier gas $H_2$
- ***Data analysis*:**
  - NIRS: partial least squares regression PLSR (R-Project)
  - EN: targeted peak detection (AlphaSoft v14)

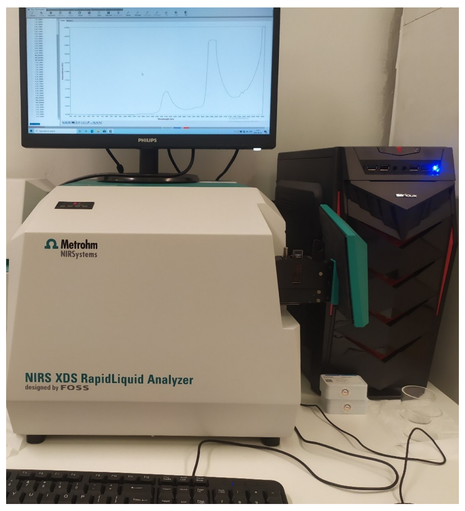

Wine samples


Model solutions



Alpha MOS Heracles Neo electronic nose


Sample preparation for EN measurements



Metrohm NIRSystems XDS NIR spectrometer with transmission cuvette (1 mm)

## RESULTS

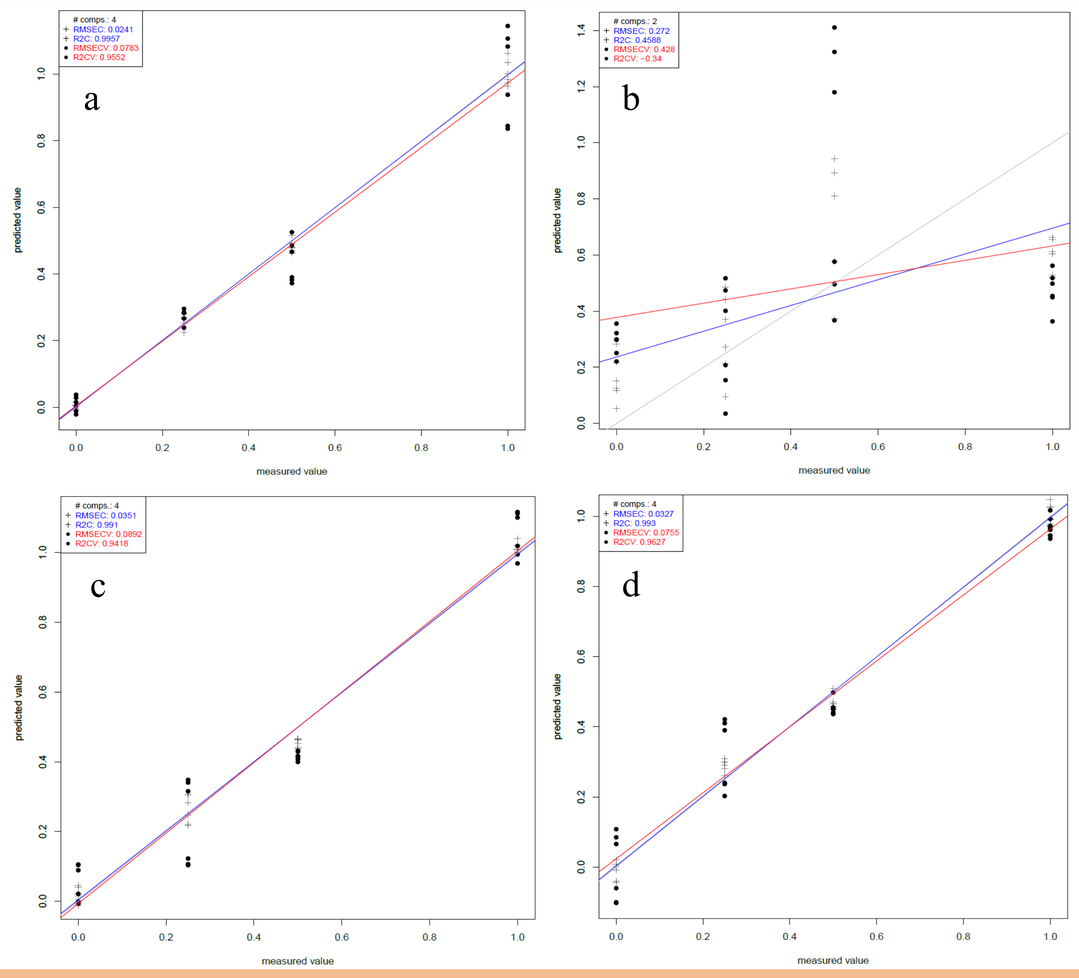



**Figure 1. NIRS results:** Y-fits, calibration and validation statistics for the AA content of Italian Riesling (a), Chardonnay (b), Cabernet Frank (c) and Pinot Noir (d) wines

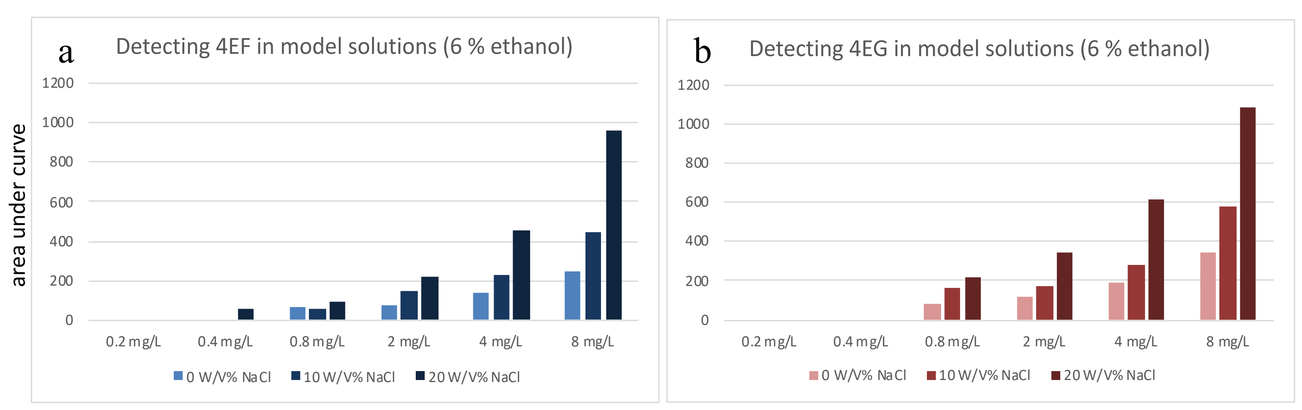



**Figure 2. EN results:** Detection of different concentrations of 4EF (a) and 4EG (b) in water-ethanol mixtures with 10 % or 20 % added NaCl; data measured with GC column MXT-5 at retention indices 1302 (a) and 1175 (b)

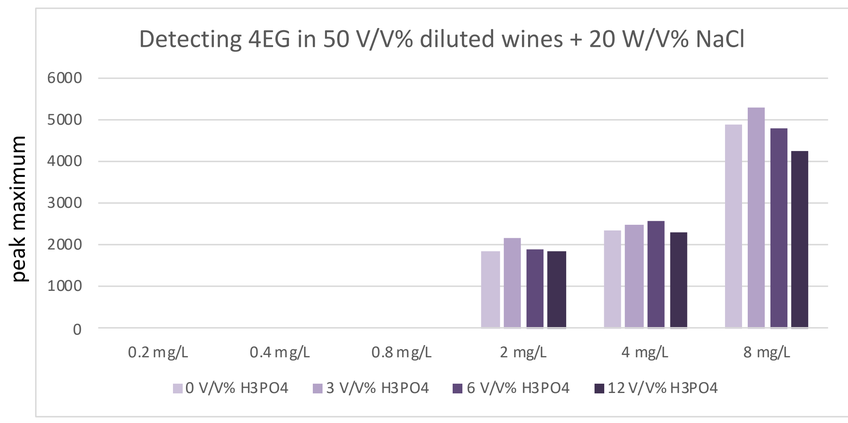



**Figure 3. EN results:** Detection of different concentrations of 4EG in diluted wine samples containing 20 % added NaCl and various concentrations of $H_3PO_4$ on top; data measured with GC column MXT-5 at retention index 1302

## CONCLUSIONS

With NIRS, 4EF and 4EG proved to be poorly estimable, however, accurate results ($R^2 > 0.9$) were obtained for AA in 3 of the 4 tested wines. The applied electronic nose was not suitable for the detection of AA, however, higher concentrations of 4EF and 4EG ($\geq 0.8$ mg/L) were detectable when the solubility of gases was reduced with addition of salt. With the addition of phosphoric acid on top, the detection limit of the targeted dissolved volatile compounds did not improve.

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