PTR-MS as a tool to optimize the performance of electronic noses

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Gas sensors vs analytical techniques

Gas chromatography
Mass-spectrometry

Chemical sensors

Tiny

Cheap

Portable

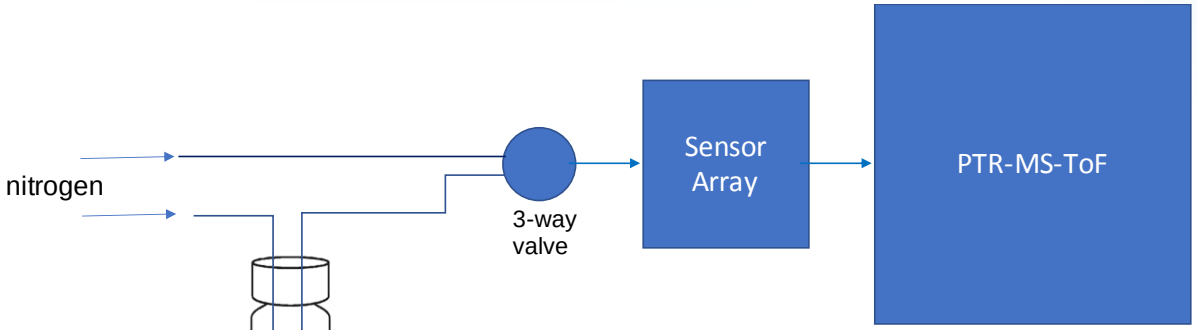
Integrable

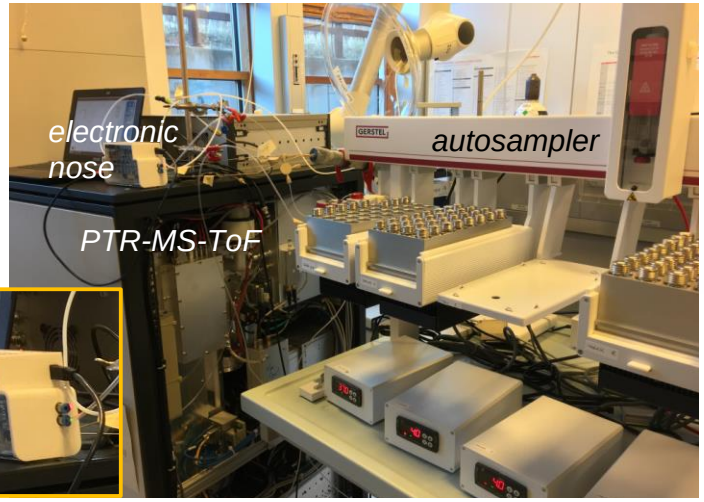
Sensitive

Recognizing

Multi-sensing

System scheme





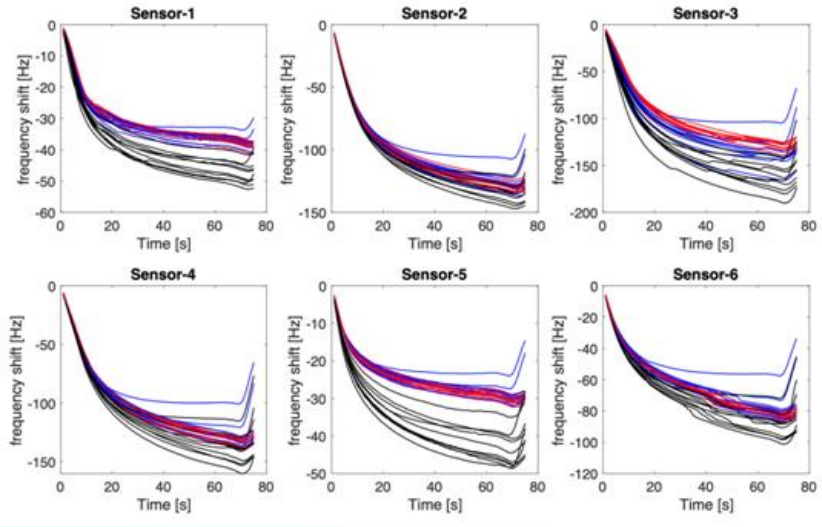
Sensors array

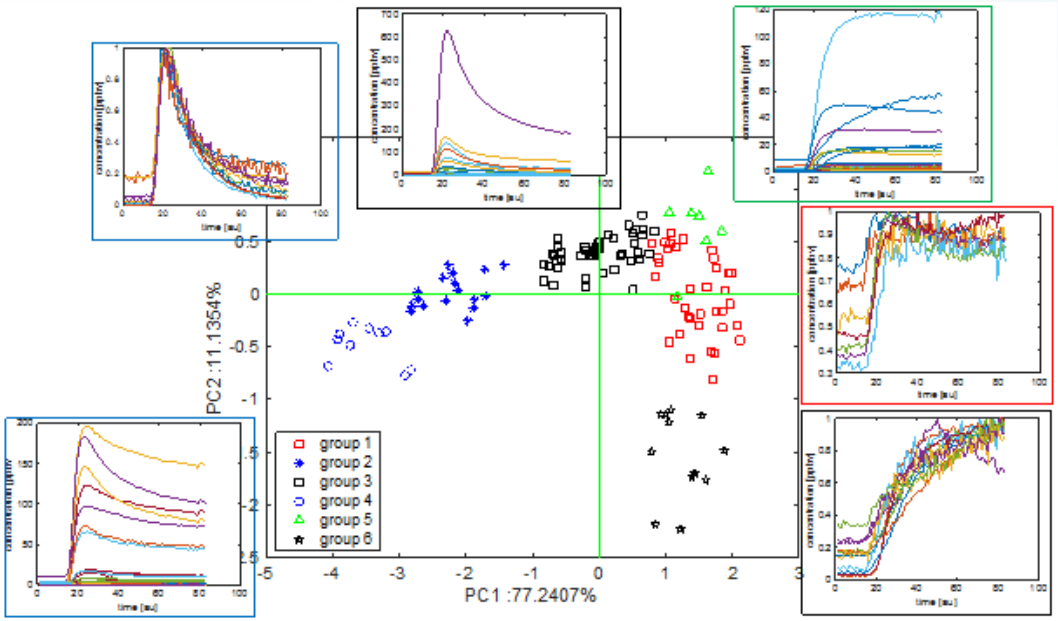
Sensors VS Proton Transfer Reaction – Mass Spectrometry

commercial tomato sauce

fresh
inoculated
+thyme oil

(Penicillium expansum, (10^6 CFU/mL))
Thymus vulgaris





sensor signal: always increasing

PTR-MS signal: different trends

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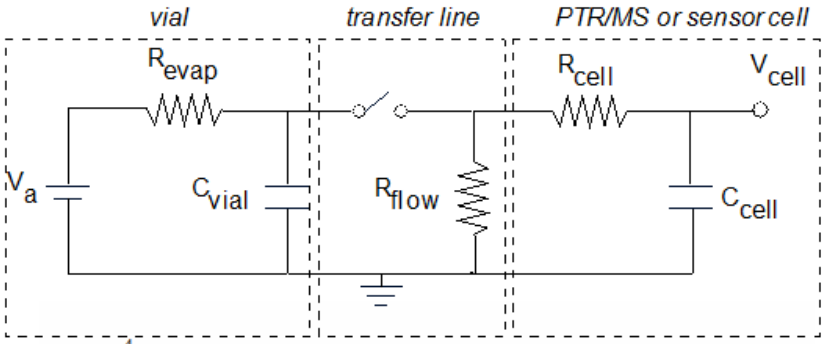
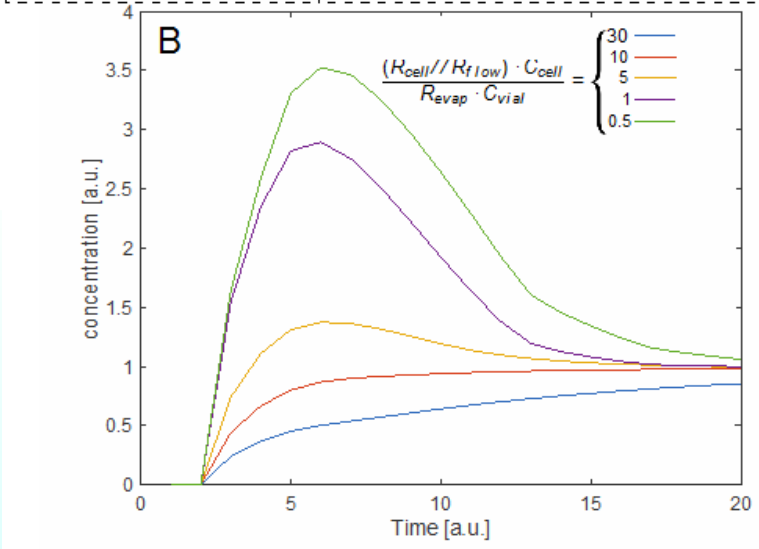
Equivalent electric circuit

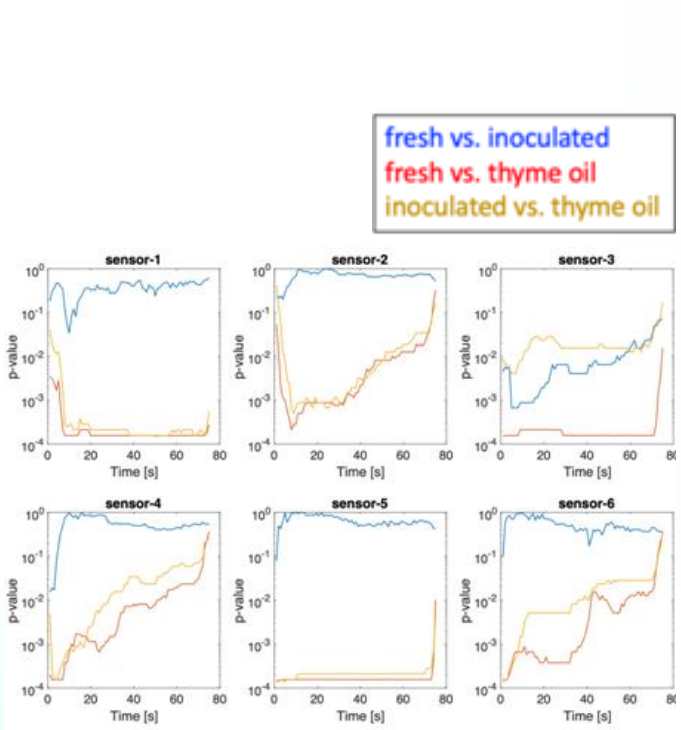




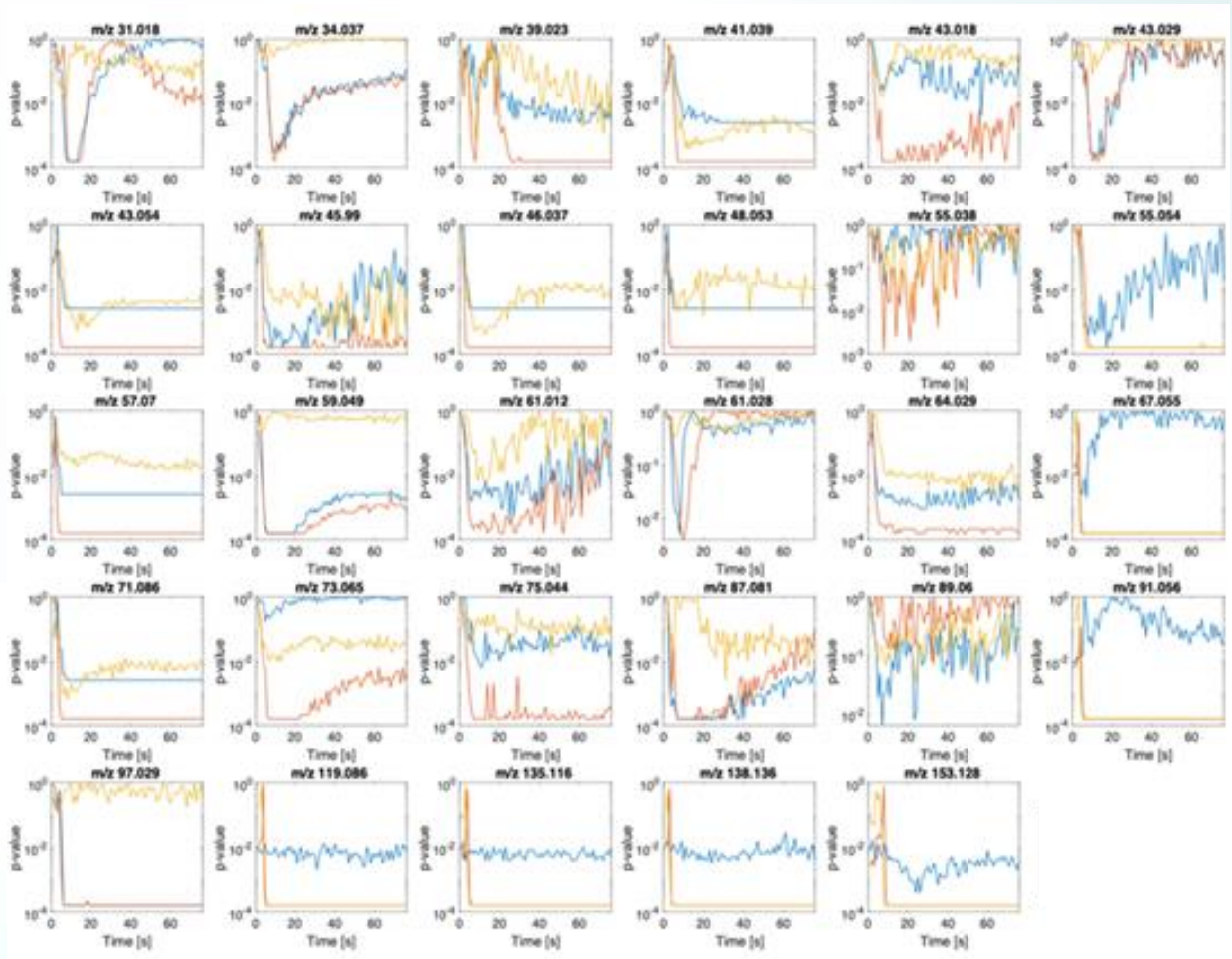
Electric quantity	Mass Transfer Quantity
Q (C)	Number of molecules (# of molecules)
I (A)	Flow of molecules (# of molecules/s)
V_A (V)	Saturation concentration (# of molecules/cm^3)
R_{EVAP} (Ω)	Inverse of evaporation volume transfer rate (s/cm^3)
C_{VIAL} (F)	Vial headspace volume (cm^3)
R_{FLOW} (Ω)	Inverse of carrier volume transfer rate (s/cm^3)
R_{CELL} (Ω)	Inverse of sensors cell filling volume transfer rate (s/cm^3)
C_{CELL} (F)	Sensors cell volume (cm^3)
V_{CELL} (V) = Q / C_{CELL}	Concentration in sensors cell (# of molecules/cm^3)

Discrimination performance

Kruskal-Wallis test



Gas sensors



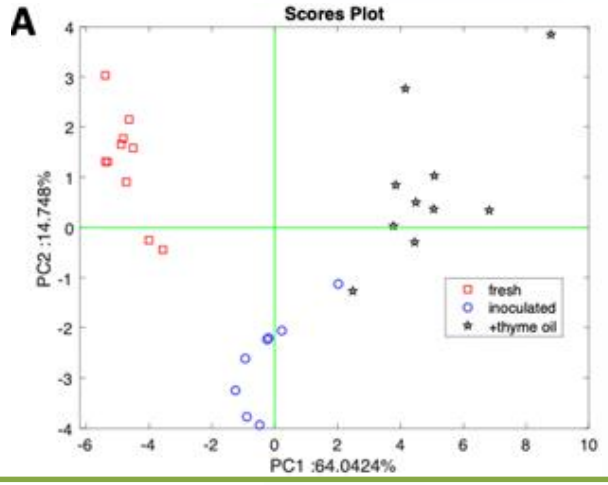
PTR-MS masses

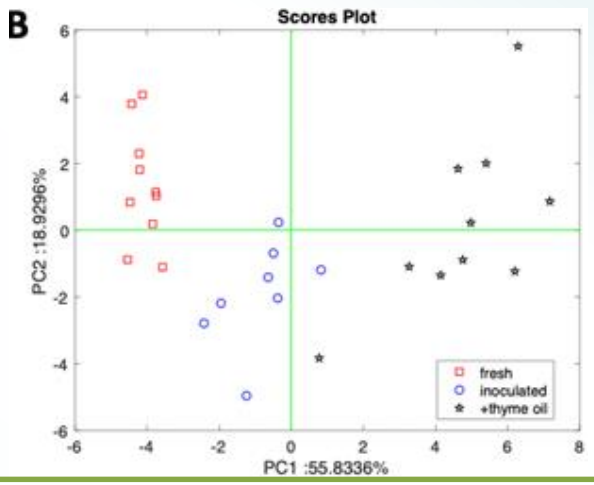
Discrimination performance

Information is constant →

PTR-MS

10 s

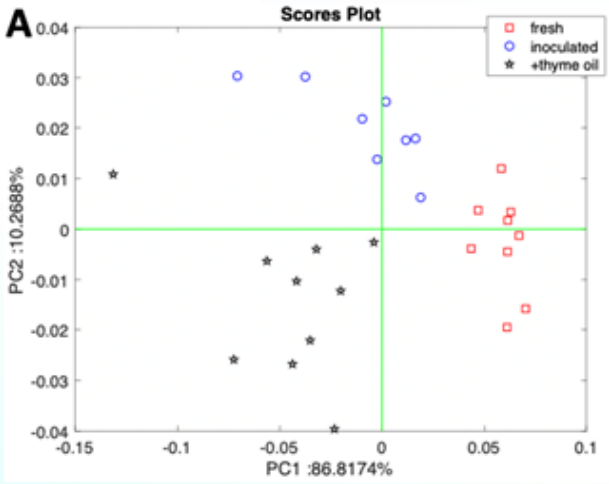


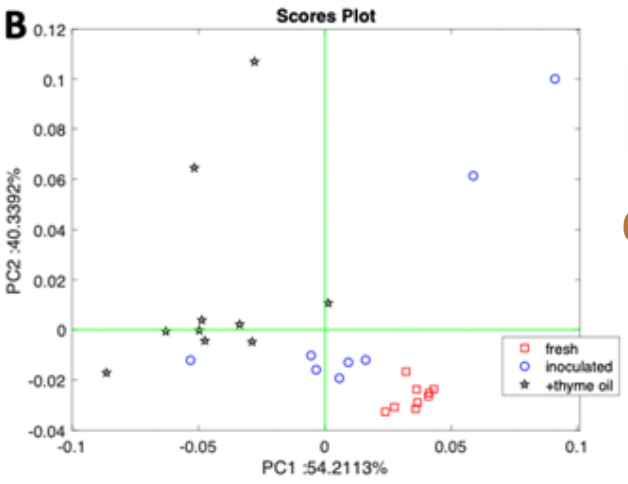


60s

sensors

10 s

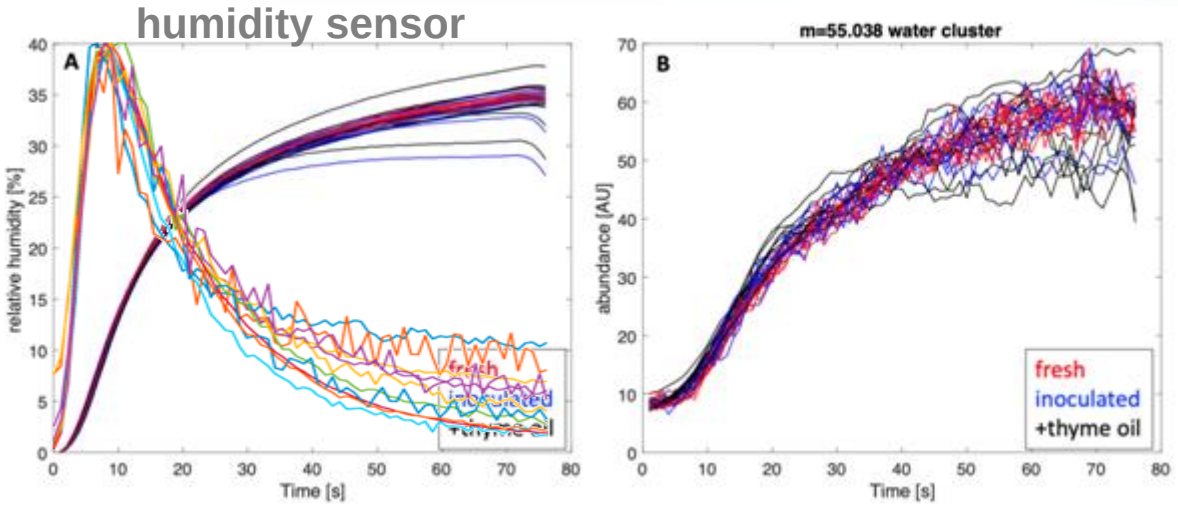




60s

Information degrades →

Why?



the culprit is… water vapor

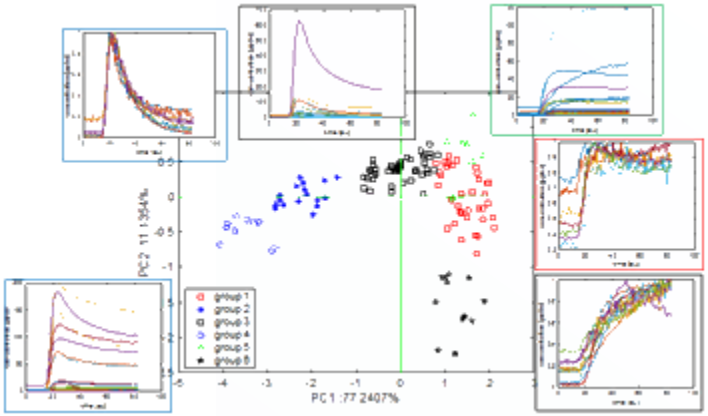
providing noise, not information

L. Quercia, I. Khomenko, R. Capuano et al.,
Optimization of gas sensors measurements by dynamic headspace analysis supported by simultaneous direct injection mass spectrometry,
Sensors and Actuators B: Chemical 347 (2021) 130580.

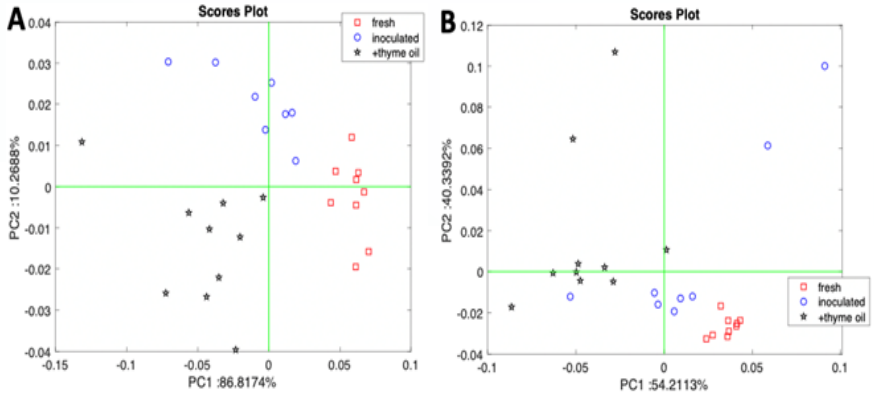
Conclusions

CSAC 2023 Chemical Sensors and Analytical Chemistry

Information and noise have different behaviors



PTRMS optimizes discrimination and gives right timing



Thin Film Materials and Nanostructure Devices for Sensing Applications

Guest Editors
Dr. Hugo Aguas
Dr. Matteo Tonezzer

Deadline
31 December 2023

Special Issue
Invitation to submit

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