



HAL
open science

A compact FT-ICR mass spectrometer coupled to a tubular oven: Analytical development and characterization

Taous Abar, H el ene Mestdagh, Jo el Lemaire, Michel Heninger

► To cite this version:

Taous Abar, H el ene Mestdagh, Jo el Lemaire, Michel Heninger. A compact FT-ICR mass spectrometer coupled to a tubular oven: Analytical development and characterization. Journ ee de la Division de Chimie Physique, Oct 2022, Paris, France. hal-03800602

HAL Id: hal-03800602

<https://hal.science/hal-03800602>

Submitted on 6 Oct 2022

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 destin ee au d ep ot et  a la diffusion de documents scientifiques de niveau recherche, publi es ou non,  emanant des  tablissements d'enseignement et de recherche fran ais ou  trangers, des laboratoires publics ou priv es.

A compact FT-ICR mass spectrometer coupled to a tubular oven:

Analytical development and characterization

Taous Abar, H el ene Mestdagh, Joel Lemaire, Michel Heninger

Institut de Chimie Physique (ICP), UMR8000, CNRS-Universit  Paris-Saclay, Orsay, France



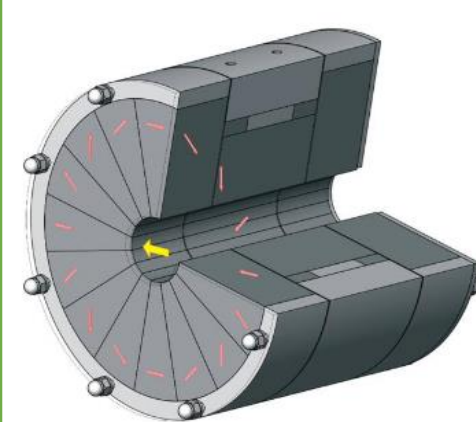
Volatile Organic Compounds (VOCs) are ubiquitous in all environmental compartments at different concentrations. More than a thousand VOCs are released by the human body in the various biological fluids (exhaled air, sweat, urine, saliva, blood...). Some VOCs excreted from our bodies may be specific for several diseases, so they can be used to reveal the presence of those pathologies.

In this work, we are interested in identifying VOC biomarkers of pathologies to establish a rapid and non-invasive medical diagnosis. To achieve this objective, we develop an analytical methodology based on mass spectrometry associated with chemical ionization by proton transfer (PTR-MS: Proton Transfer Reaction - Mass Spectrometry). The proton transfer reaction allows a very selective ionization of VOCs, which facilitates their quantification and identification thanks to the high resolution of the mass spectrometer.

Compact FT-ICR mass spectrometer « AQUAREM »

- Ion trap and mass analyzer with permanent magnetic field
- Chemical ionization in positive/negative mode or electron impact
- Analysis of VOCs in Liquids and gases
- Mass range 4 => 150 u with a resolution of 10000 @m/z 19

HALBACH structure: 3 cylinders each one is divided in 16 segments



The magnetic field is 1.2 T



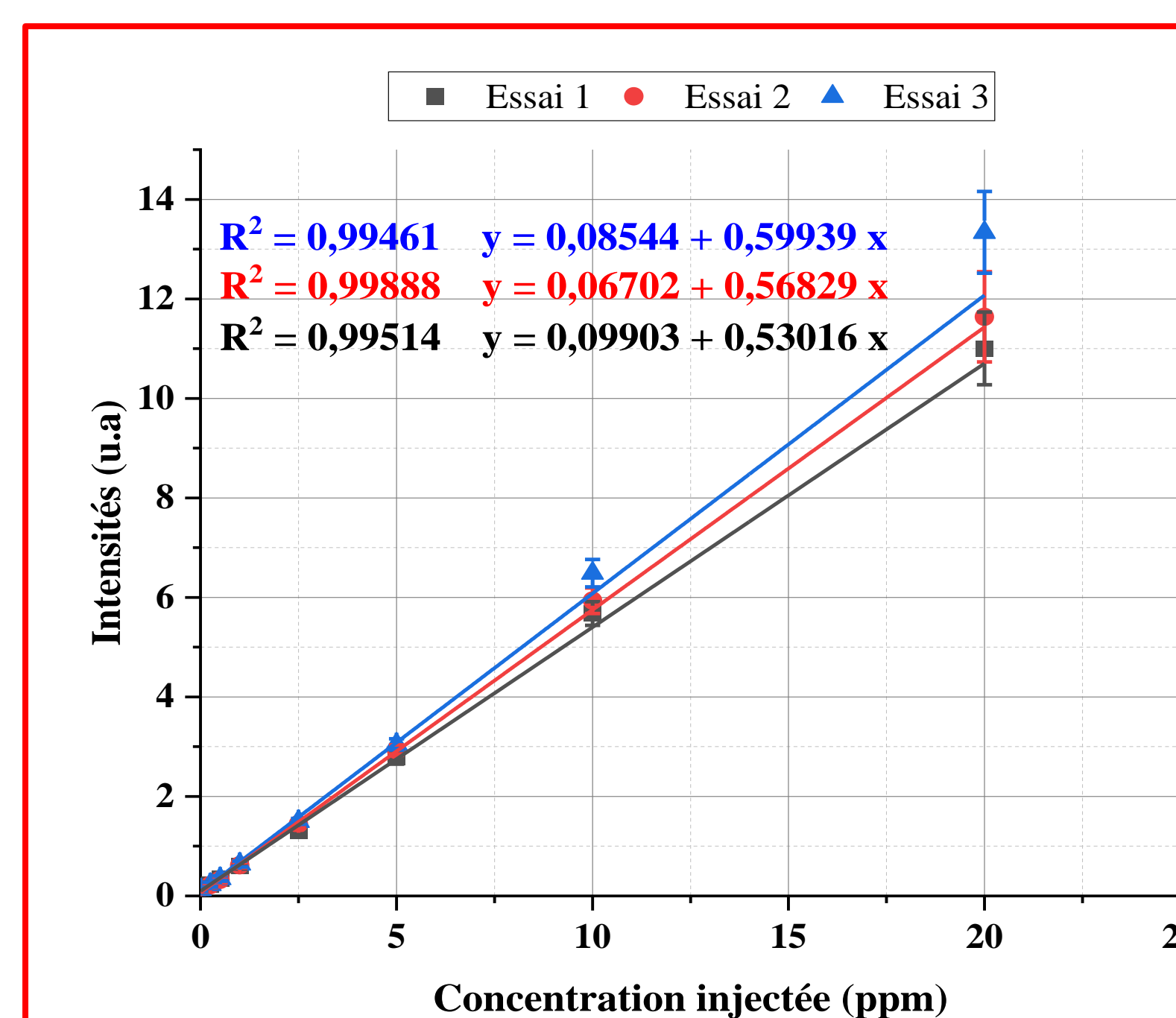
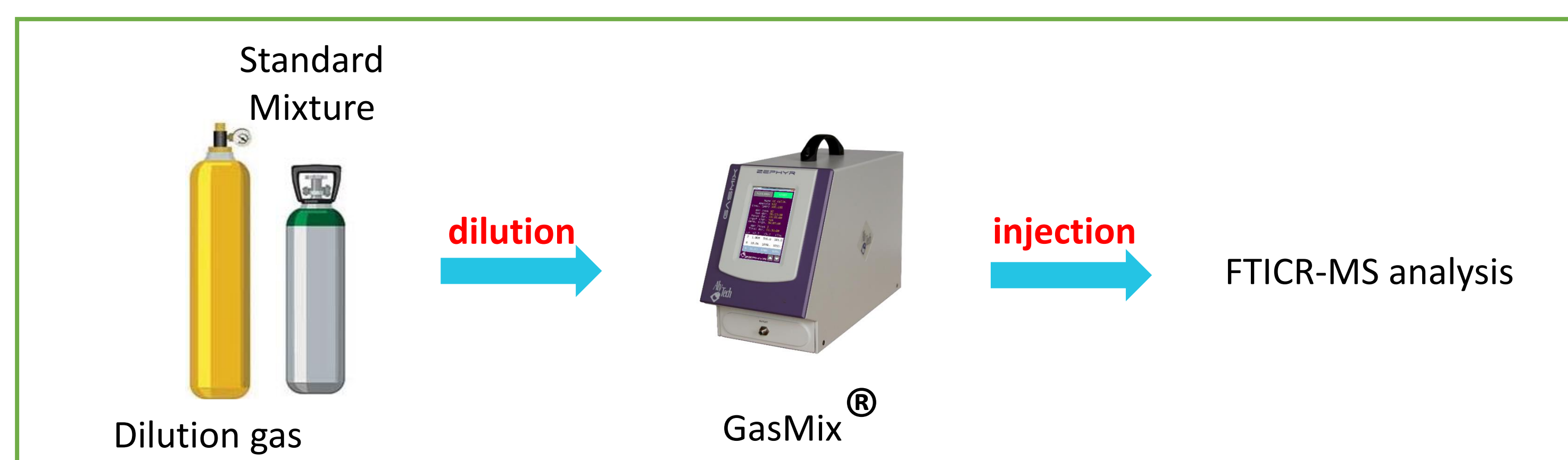
The cell features 3 sections and is open on lateral sides for better pumping

Trapping electrodes of the central section divided into 5 segments for a linear excitation

Chemical ionization:

- Soft ionization => Almost no fragment
- Very selective => No reaction with the matrix
- Absolute quantification if the reaction rate coefficient is known
- VOCs ionized by proton transfer: $H_3O^+ + VOC \rightarrow H_2O + (VOC)H^+$

Determination of the LOD using diluted gases

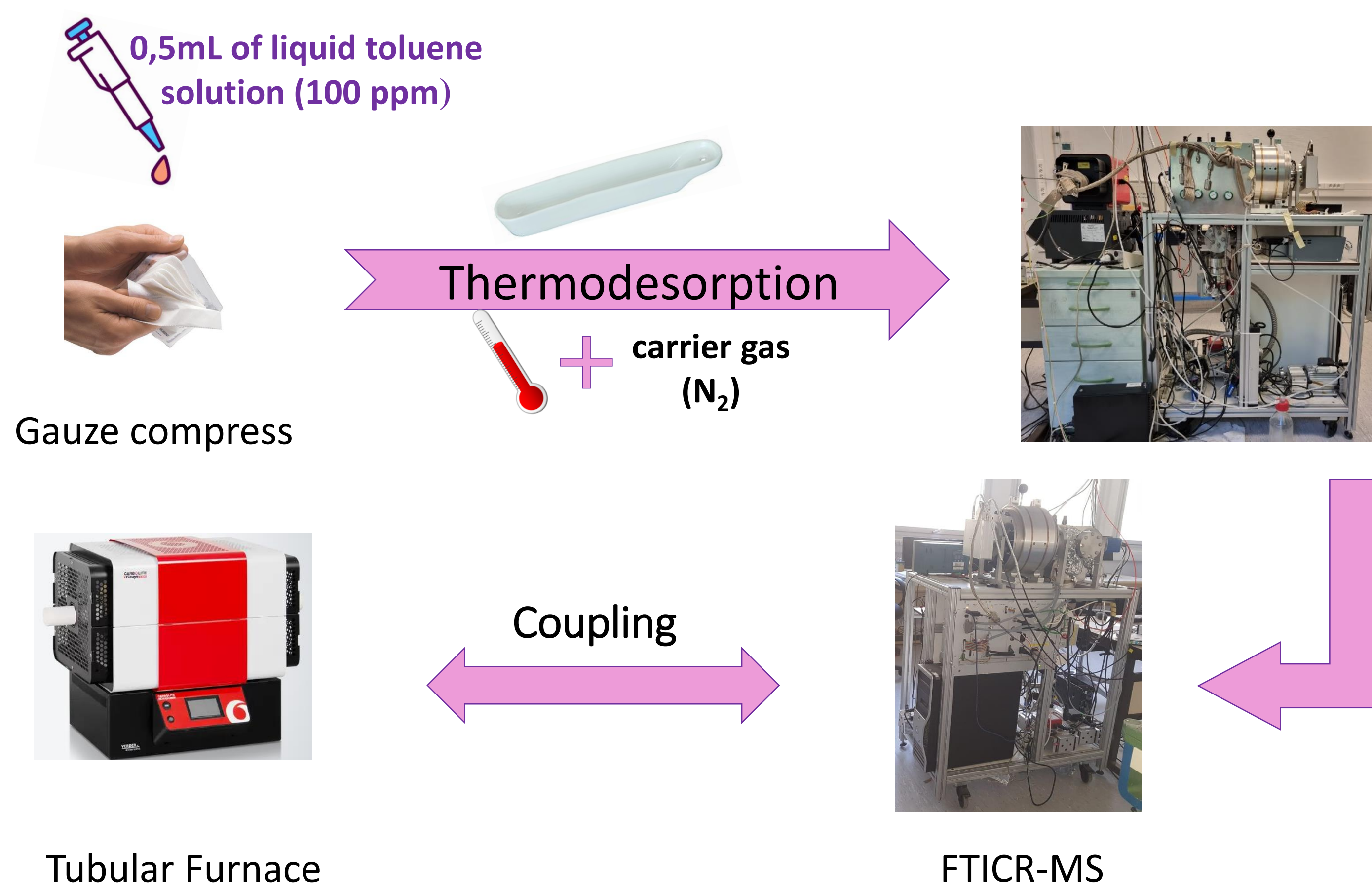


To check the detection linearity, The concentration of analyte is varied, here from 250 ppb to 20 ppm by changing the dilution in the air matrix

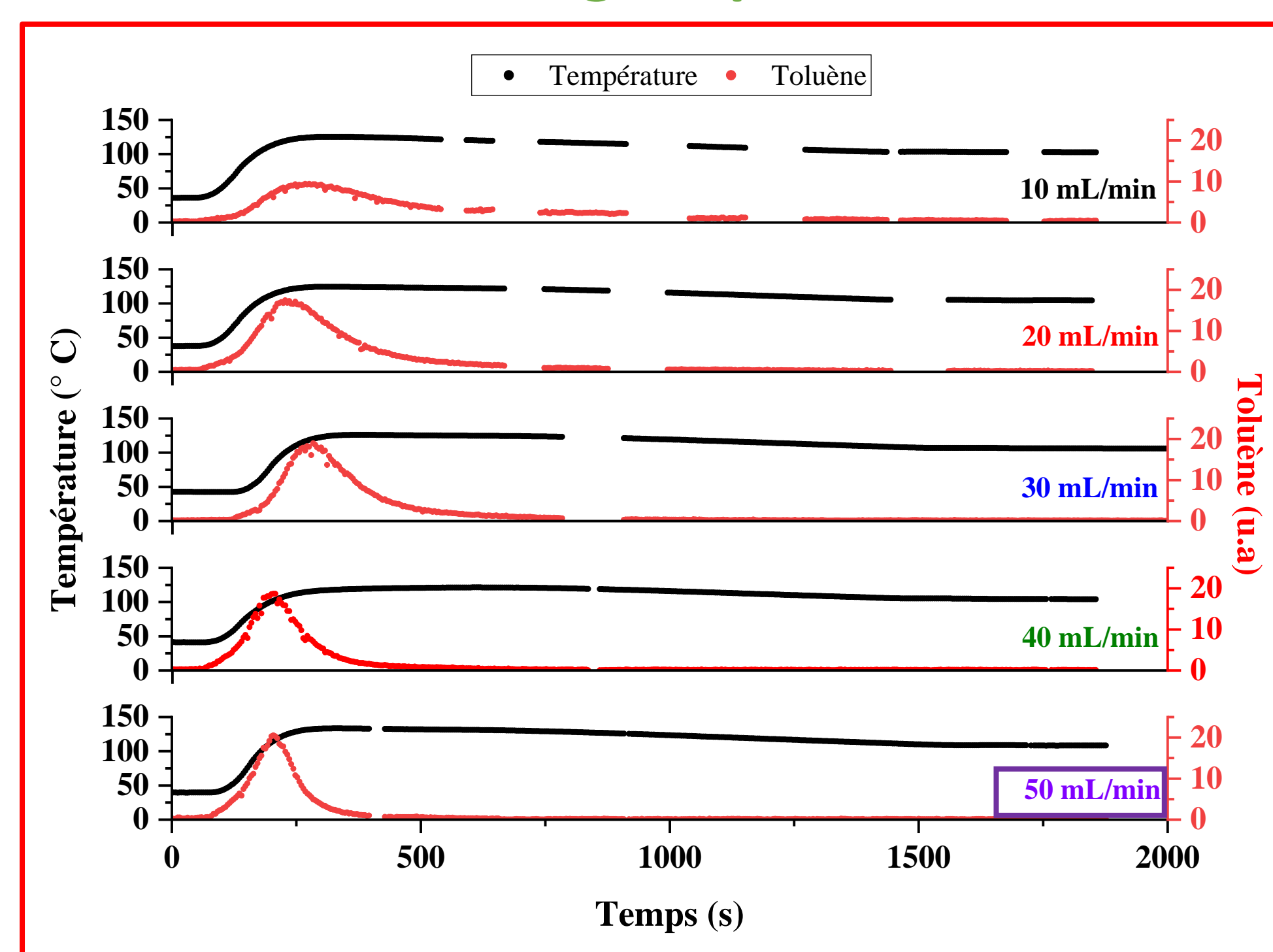
Analytical instrument linearity is verified

The LOD (Limit Of Detection) found for toluene is: 250 ppb

Coupling the FT-ICR AQUAREM with a tubular oven



The flow of carrier gas optimization

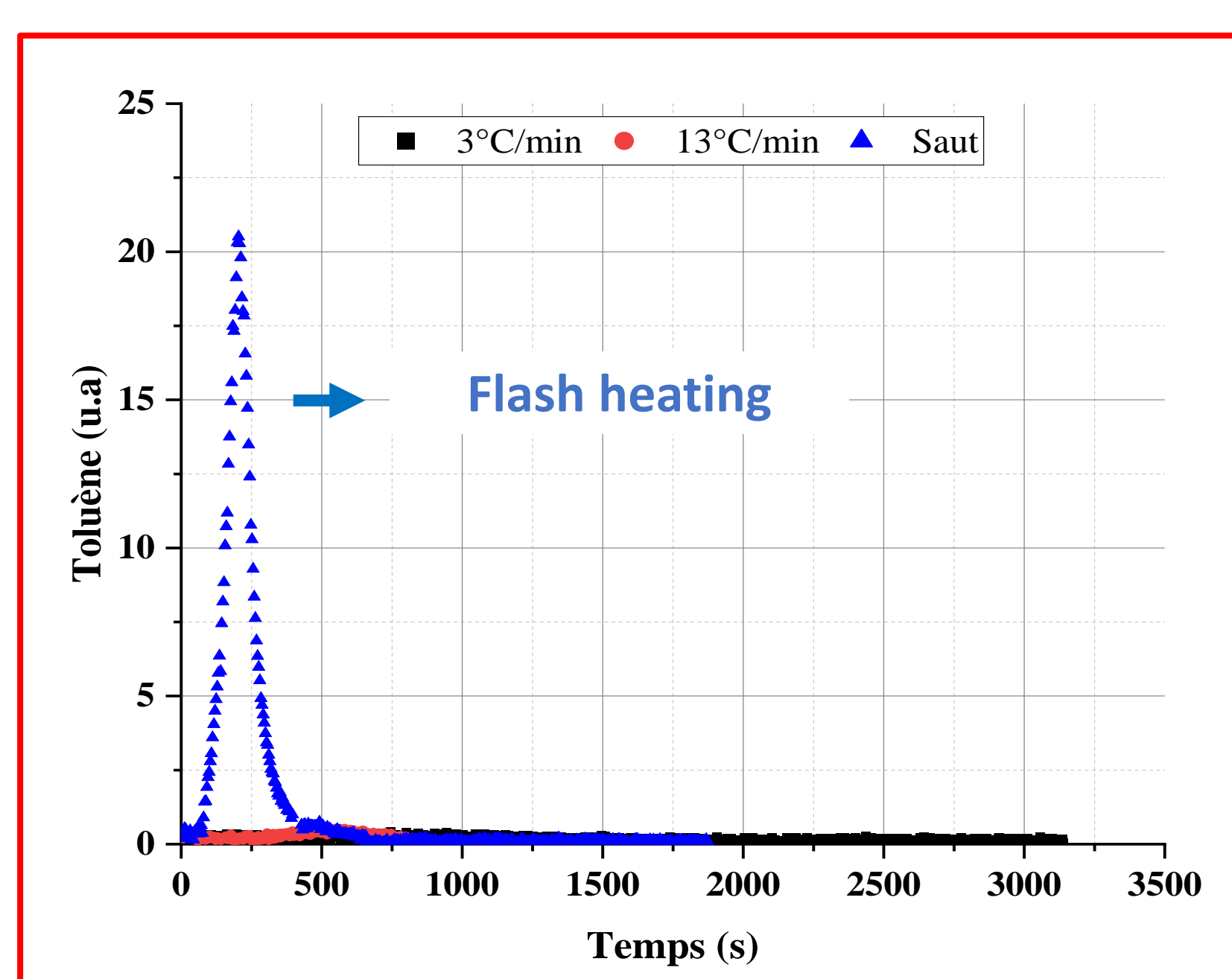


05 gas flow values of carrier gas

Flash heating (150  C)

Peak characteristics

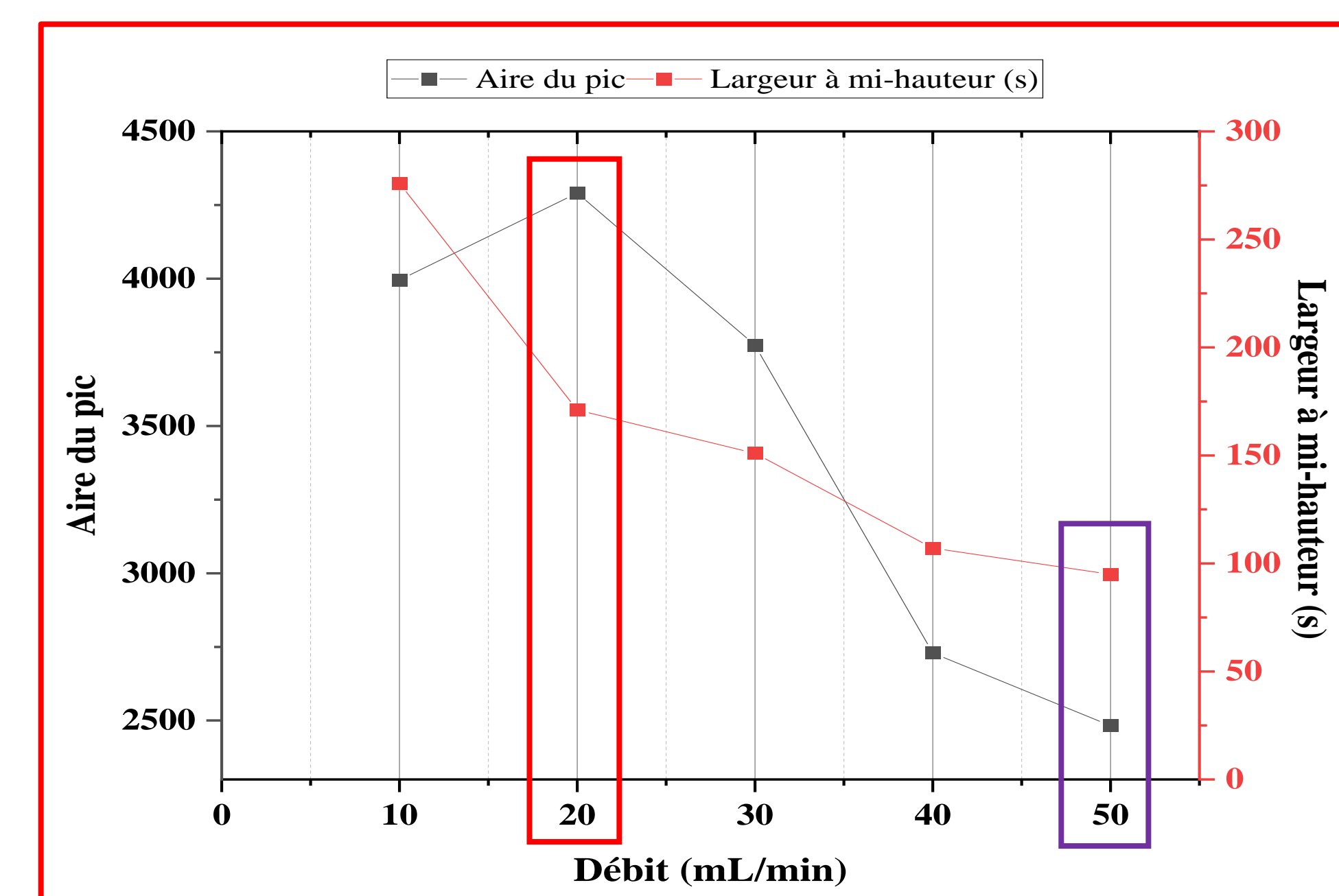
Heating program optimization



Flash heating from 35  C to 150  C gives the best intensities

For 50 mL/min the peak is thin

for 20 mL/min the peak's area is maximal



Conclusion and prospects

- Soaked volume optimization
- LOD determination and validation of linearity of significant VOCs
- VOCs mixture analysis