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# Real time analysis at high resolution with a small FT-ICR mass spectrometer

Julien Leprovost<sup>1</sup>, Gérard Mauclaire<sup>1</sup>, Pierre Boissel<sup>1</sup>; Joel Lemaire<sup>2</sup>, Michel Heninger<sup>1,2</sup>,

<sup>1</sup>ALYXAN, Centre Hoche, 3 rue Condorcet, 91260 Juvisy sur Orge, France.

<sup>2</sup>LCP, CNRS-Université Paris-Sud, bât. 350, Centre Universitaire d'Orsay, 91405 Orsay Cedex, France .

## Introduction

**Real-time and on line monitoring** of complex mixtures is a crucial need for industrial and environmental analysis. Mass spectrometry can play a role in this field if the compounds can be identified and quantified.

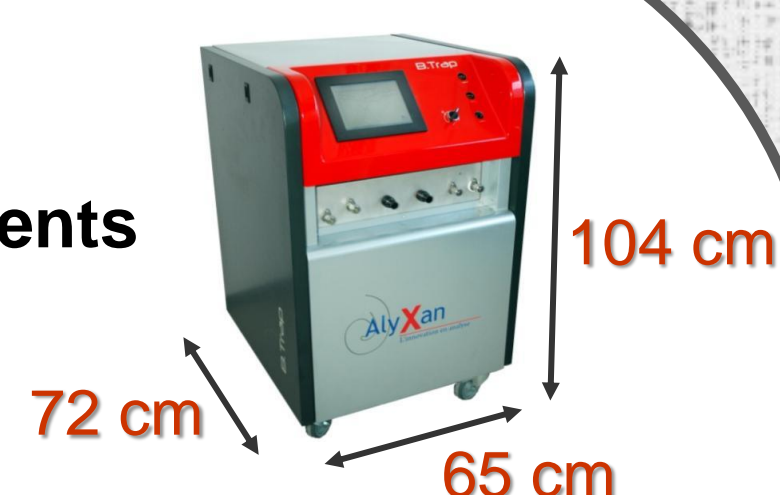
When separation techniques like gas chromatography are too slow to be used, identification and quantification of the compounds can be done with our mass spectrometers using a soft ionization technique followed by a precise mass measurement of the resulting ions.

The solution developed by AlyXan associates Chemical Ionization (CI) with a new compact FT-ICR (Fourier Transform Ion Cyclotron Resonance) mass spectrometer: BTrap.

Compared to quadrupole analyser, the use of FT-ICR brings specific and significant advantages for mass detection: (i) mass measurements precision 0.01u, (ii) mass resolution allowing isobaric separation, (iii) broad band detection; the whole mass range (10-300) is recorded in less than 1 sec.

## Instrumentation

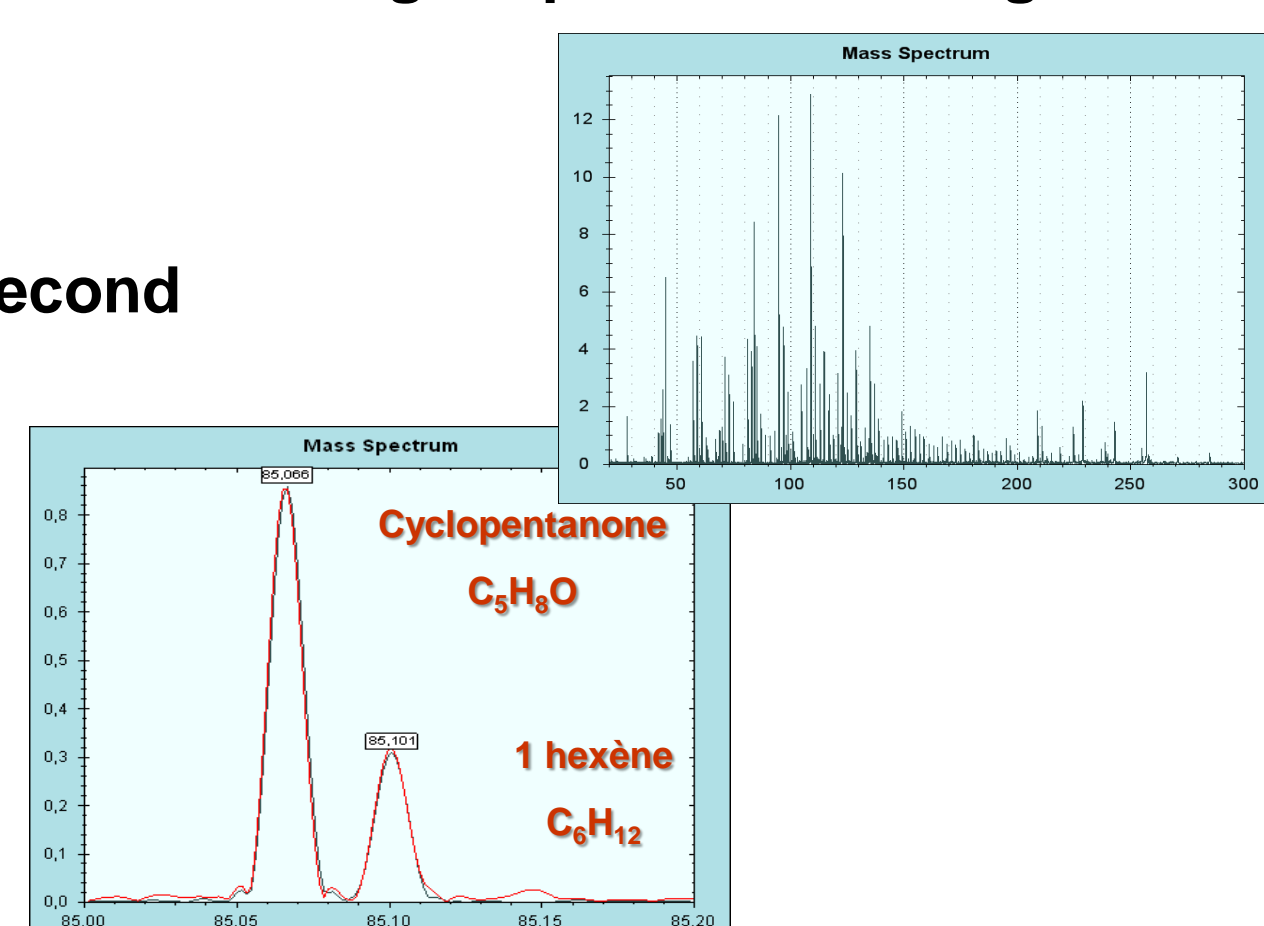
### Compact FT-ICR mass spectrometer instruments



AlyXan has been developing compact FT-ICR mass spectrometers for several years. The originality of AlyXan's instruments is in the use of permanent magnets to produce magnetic fields. The instrument is based on a permanent magnet: Hallbach cylinder. The field obtained is perpendicular to the bore of the cylinder with a value of 1.5 Tesla.

The instrument is **compact and mobile** and simply requires an electric plug for activation. Compared to a quadrupole analyser, the use of FT-ICR brings **specific and significant advantages** for mass detection:

- **Broadband detection: full spectra in just one second**
- **High resolution: precise mass determination**
- **Isobaric separation**
- **Ion Trap: allows several mass selections (MS<sup>n</sup>)**



### Transportable, rugged



Air measurements in a purifying station



Air monitoring in a confined space

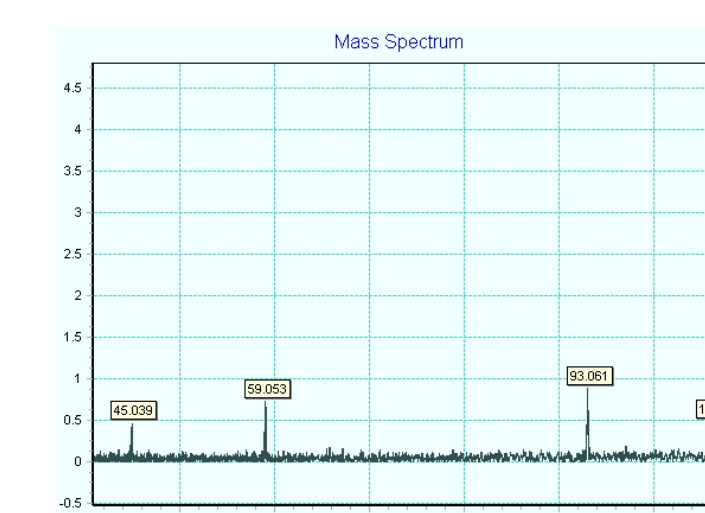
## Chemical Ionization

Chemical ionization is a selective, soft and quantitative technique for analytical applications. For analysis of Volatile Organic Compound (VOC) emissions, Proton Transfer Reaction Mass Spectrometry (PTRMS), which has proven its efficiency, was used. For example proton transfer reaction from H<sub>3</sub>O<sup>+</sup> is quite fast and the rate constants are well known allowing excellent quantification of the traces.



With a direct pulsed injection of air in the trap, traces can be detected in real time (<1s) from 200 ppb to few % with a linear response.

Example: acetaldehyde, acetone, toluene, xylene in air (ppm level) :



4 compounds  
4 peaks!!!

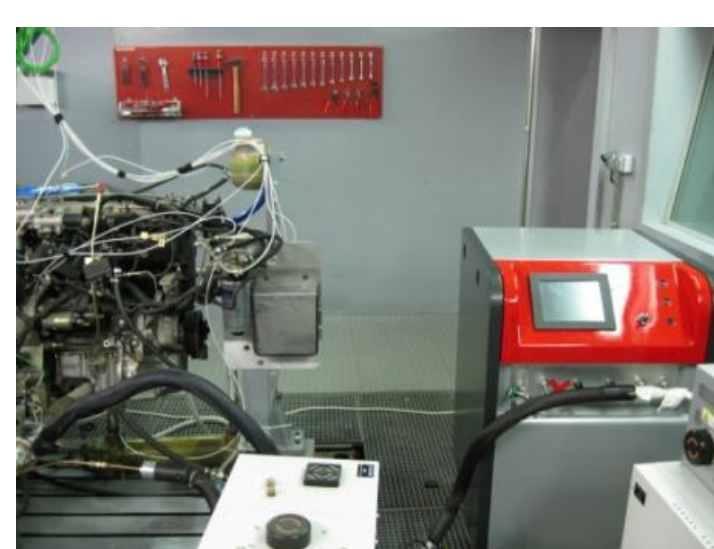
Since the ions are trapped in the ICR cell, this technique is also very convenient for the use of chemical ionization. Successive steps including mass selections, ion-molecule reactions can be performed inside the cell, allowing the use of a wide variety of reactant ions: positive ions; Xe<sup>+</sup>, O<sub>2</sub><sup>+</sup>, NO<sup>+</sup>, CF<sub>3</sub><sup>+</sup> or negative ions; O<sup>-</sup>, OH<sup>-</sup>.

Using MIMS (Membrane Inlet Mass Spectrometry), the sensitivity goes down to the ppb levels with a response time shorter than 60 s.

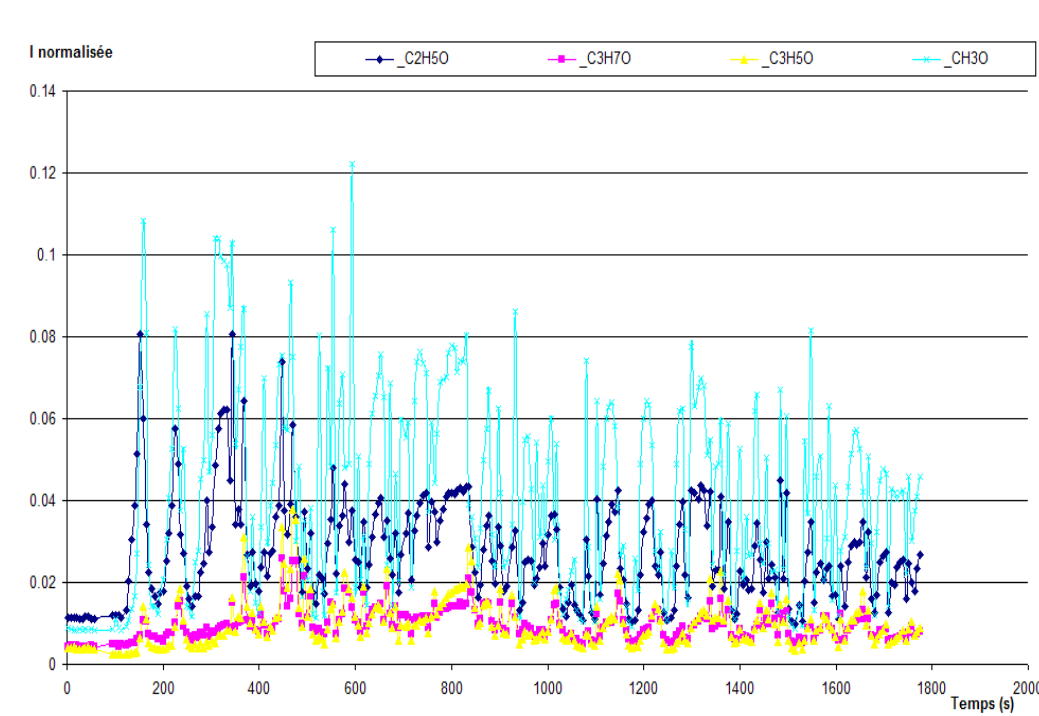
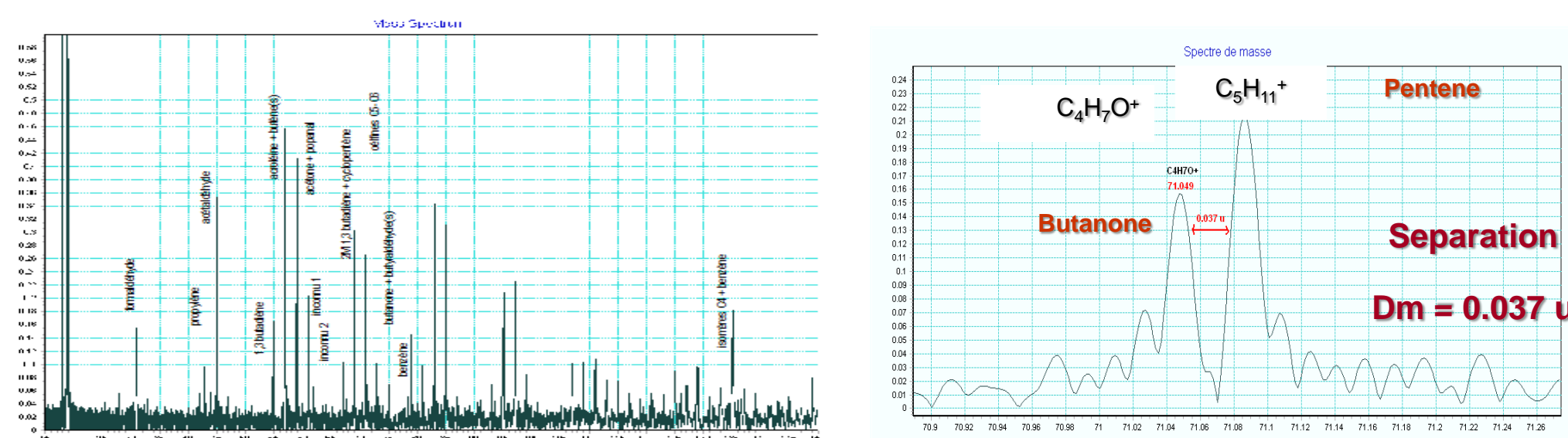
## Car exhaust emissions: Engine testing for biofuels

**Objective** : On-line measurements of regulated compounds (NH<sub>3</sub>, NO) or unregulated compounds (VOCs).

High resolution is important to separate: O (15.9949 u) and CH<sub>4</sub> (16.0313u).



Engine test: Artemis (Euro 6)

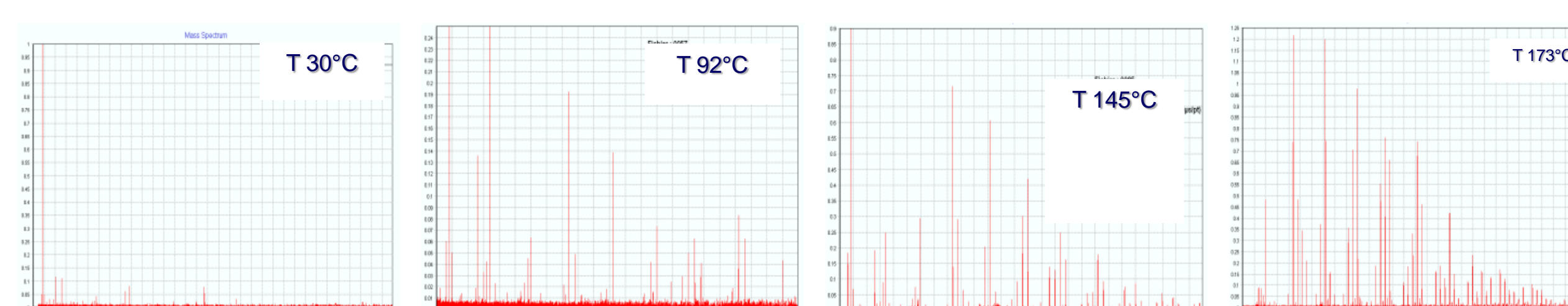


Fast monitoring of VOCs emissions

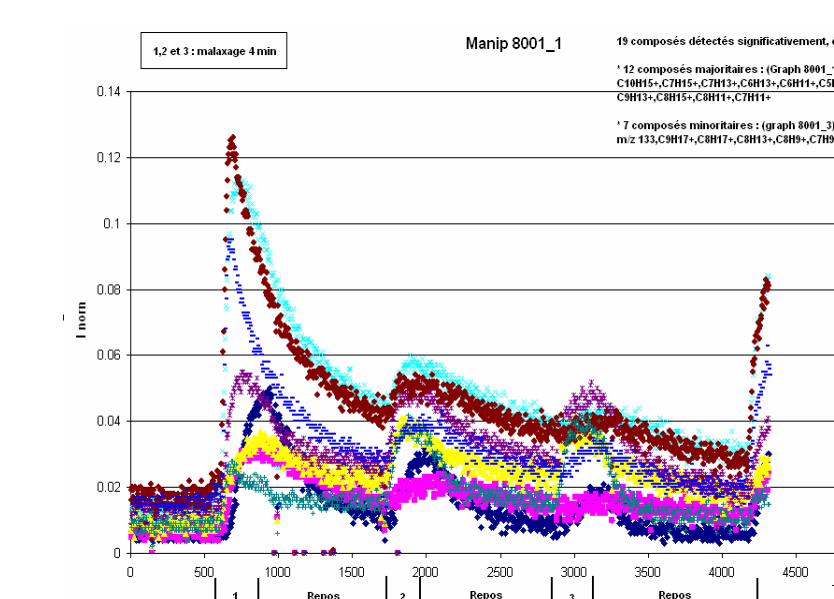
## Headspace of hot bitumen

Hot bitumen products may give off irritant fumes

Real-time analysis, varying mixing stage and temperature



Simulation of the different steps of bitumen preparation: from production to its application on the road.



## Key points:

High resolution mass spectrometry coupling with Chemical Ionisation is **well suited for real time analysis of organic compounds.**

Contact: [julien.leprovost@alyxan.fr](mailto:julien.leprovost@alyxan.fr)

Tel: +33 (0)1 69 96 95 19

- Real time analysis (1s to 1min)
- Large band detection: full spectrum in one second
- Quantitative analysis
- High resolution: determination of molecular formula.
- On site
- Multiplexing of several sampling lines

## Applications:

- Industrial processes
- Indoor pollution
- Industrial emissions
- Material degradation