



# Real time gas phase puff-by-puff profile

## Gas phase Fingerprint of specific filtration

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# Motivation

- **Real time** - fresh cigarette

*toxicity assessments : chemical composition of particles in mainstream as well as in their distribution in different size fraction*

- **Puff/Puff** - dynamic information

*NTM/burning tobacco interactions  
the most fascinating techniques*

- » Multiplex GCMS/  
GCUV DAD
- » SPI-TOFMS

- **High throughput screening method**

*for PREPs development  
using a commercial system*

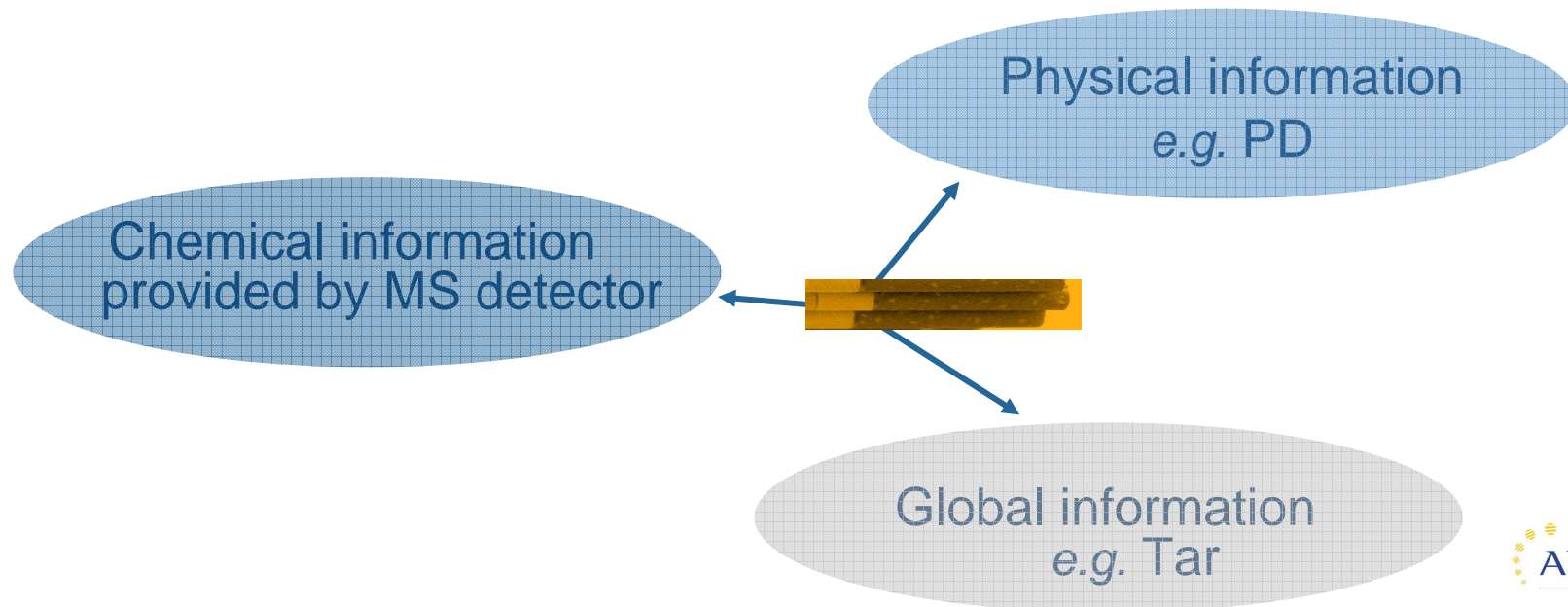
# Objective

- Screening technique

- Strategy

Step 1 -without dilution or interface materiel (gas bag, teflon vessel, gas washing bottle), find a high throughput system to compare gas phase of smoke products for NTM screening studies.

“as simple as possible, but not simplistic”



# Proper Goals

- Sampling and detection capabilities
- Tests instrumentation    precision, sensitivity  
   data processing
- Works in conjunction with NTM screening

# Experimental set-up

## ■ Characteristics

- a modified 5973N mass selective detector
- a specific two-stage gas interface
- a control/monitoring software



*The Agilent 5000A  
Real-Time Gas Analyzer.*

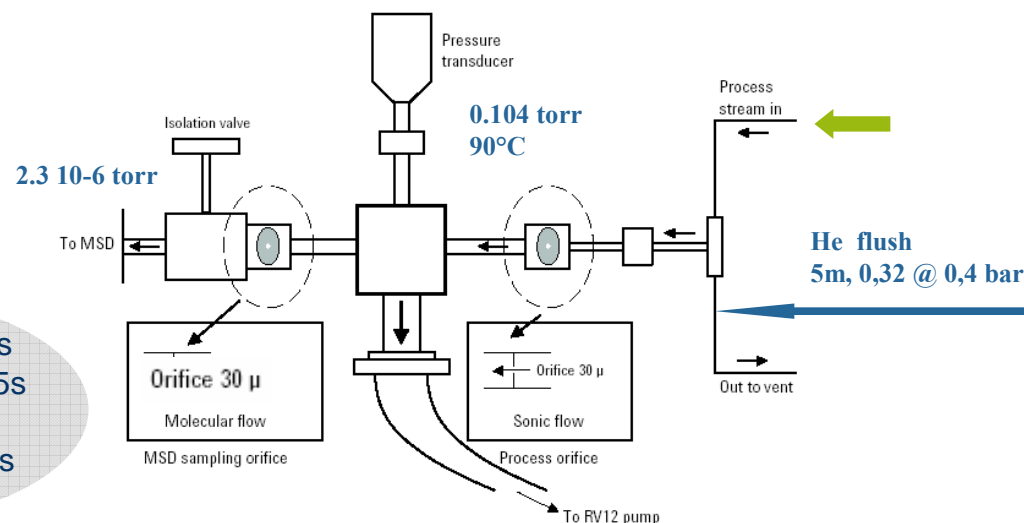
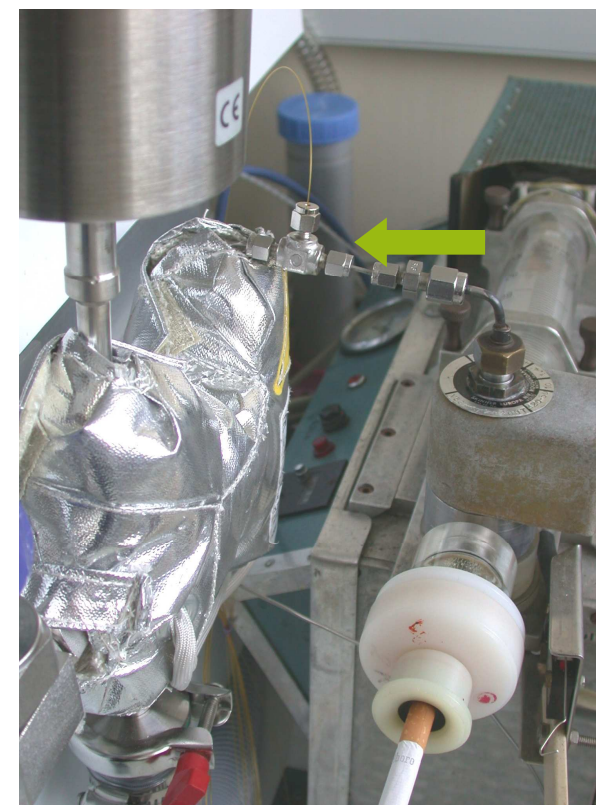


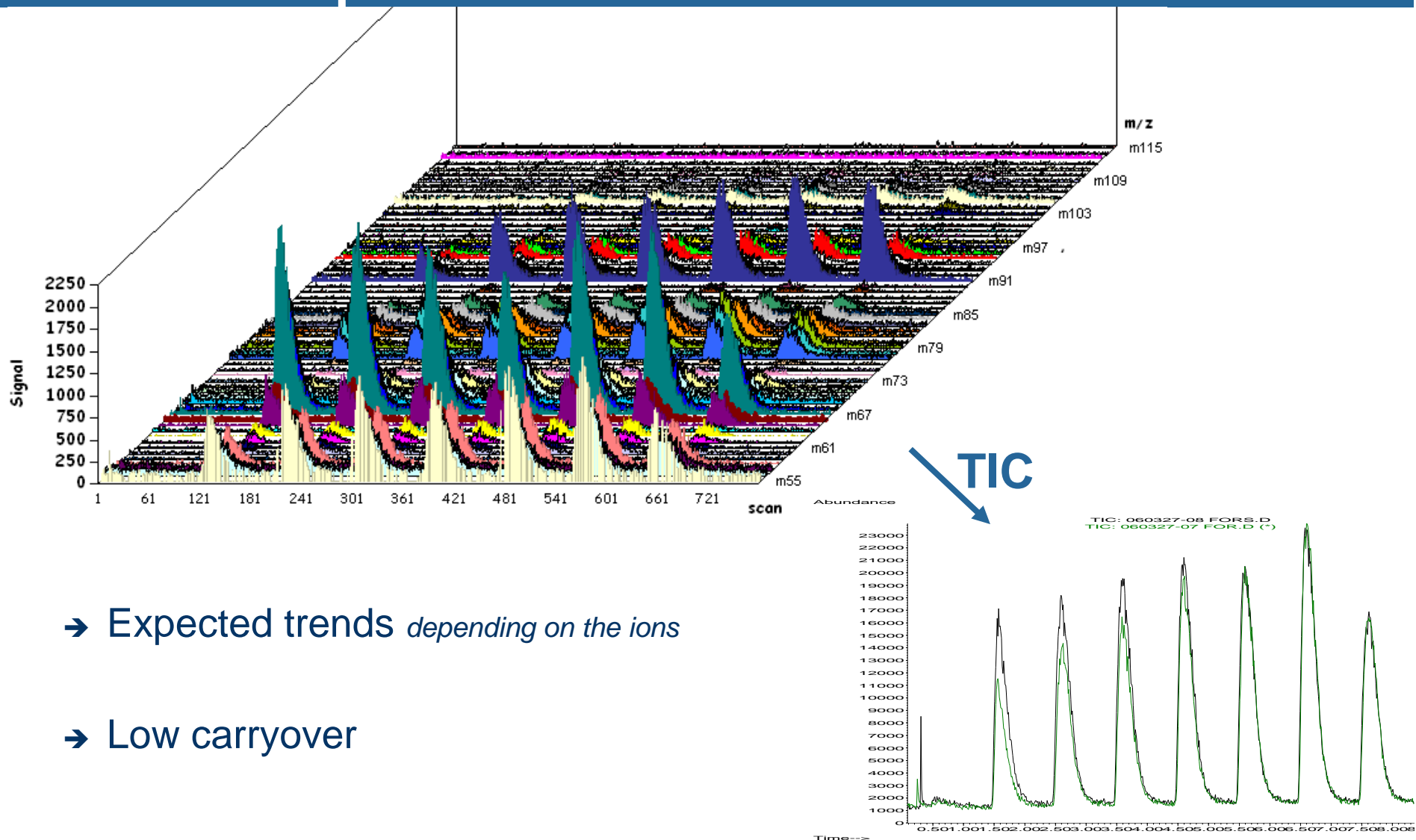
Figure 1. Diagram of the RTGA gas interface.



scan / SIM modes  
Response time 2-5s  
R~ 1 amu.  
Dwell time 500 ms

## ■ An easy-to-operate intuitive system

# Puff/Puff profile



- Expected trends *depending on the ions*
- Low carryover
- Main drawback : use of glass filter fiber

# Reproducibility, sensitivity

## ■ Precision

2R4F results

	RDS (%)		
	day 1	day 2	day 3
	N=5	N=5	N=5
TIC	5.3	6.3	4.1
m/z 92	8.0	7.0	5.1

## ■ Desired sensitivity obtained

VOC as an indicator

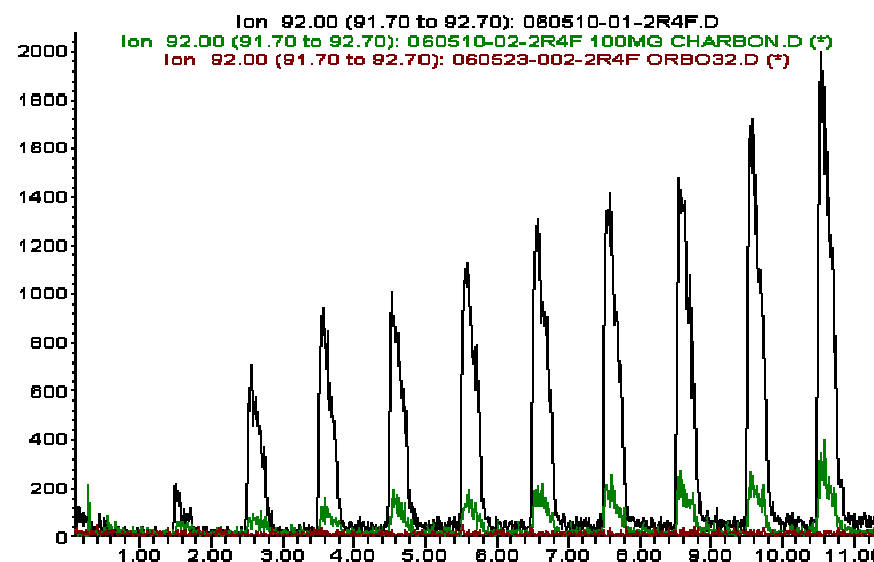
Hoffmann quantification and m/z 92 profile

Toluene =  $73.4 \pm 4.3$  µg/cig

Toluene =  $4.6 \pm 0.4$  µg/cig

Toluene < 2.0 µg/cig

Abundance



Time-->



# Sensitivity & Comprehensive data

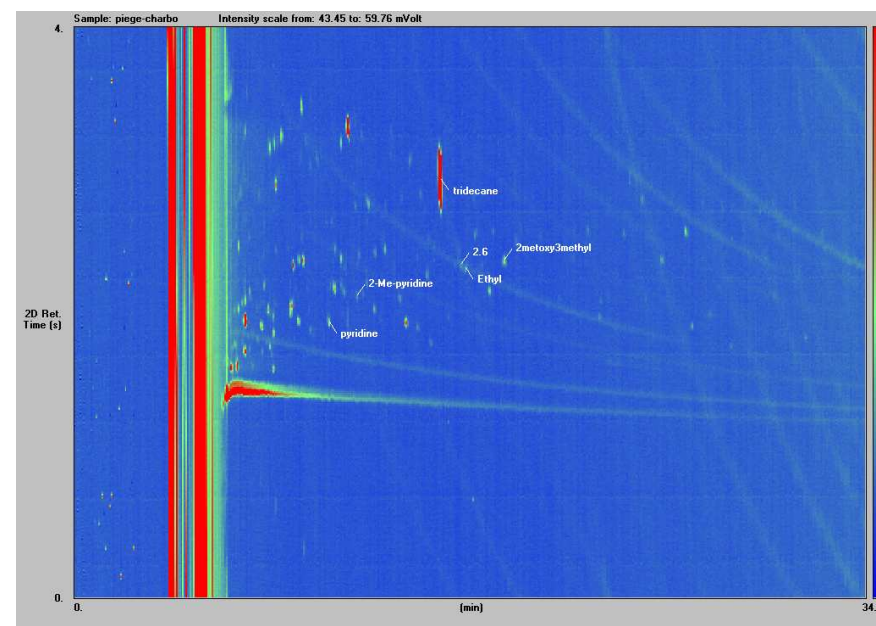
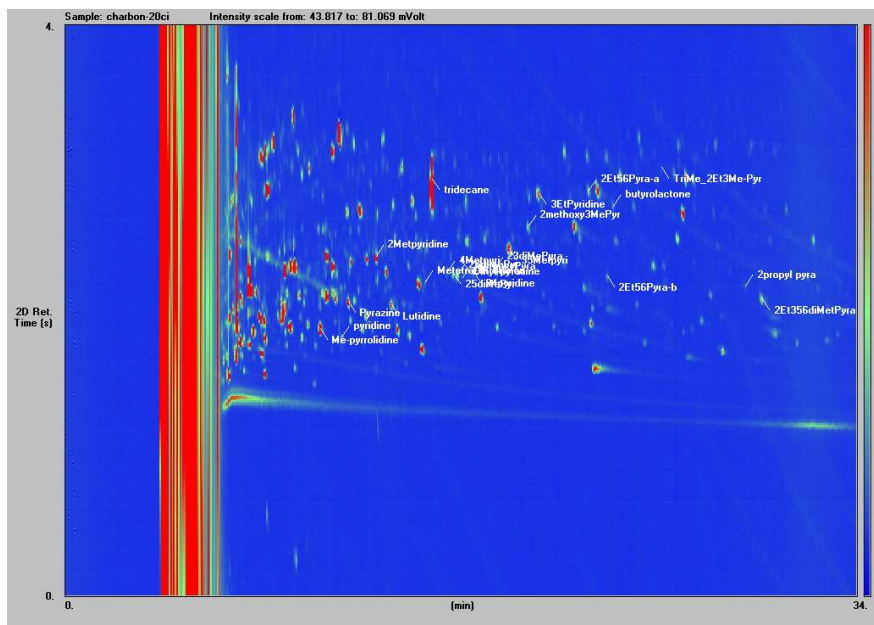
## ■ Gas phase GCGC profiles

Sol Gel Wax (30m\* 0.25mm\*0.25 $\mu$ m) X Rtx\_1701 (1m\* 0.1mm\*0.1 $\mu$ m)

Low VOCs levels (Toluene < 2.0  $\mu$ g/cig)

RTGA smoking conditions (1 cig.)

ISO smoking conditions (20 cig. on RM20SCR)



RTGA over a broad range of volatile compounds screening up to m/z 115



# Specificity ?

## ■ Limitations

- Specificity : not expected because we are looking at mass fragments at 70eV.
- Individual Puff results : not very comparable because we are looking on different partitioning due to the filter desorption.

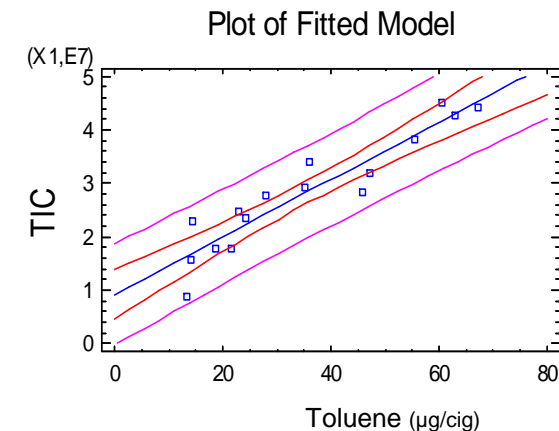
## ■ Nevertheless

- relationship between TIC (RTGA) and Toluene (Hoffmann quantification)

*Screening on Different Adsorbents*

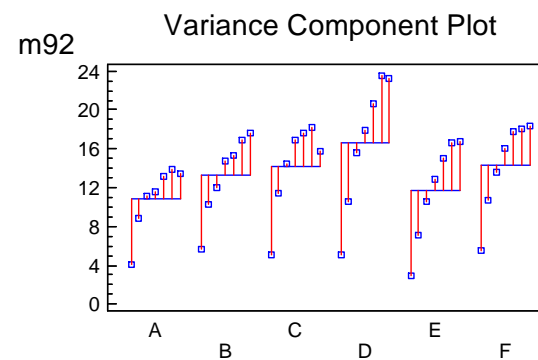
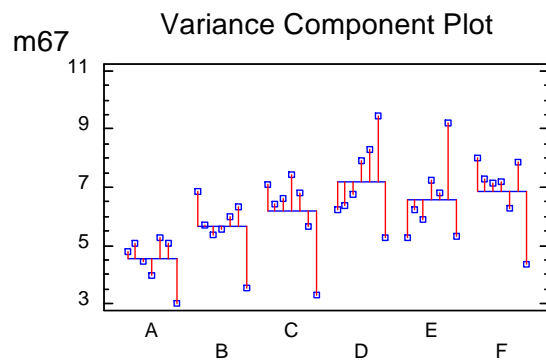
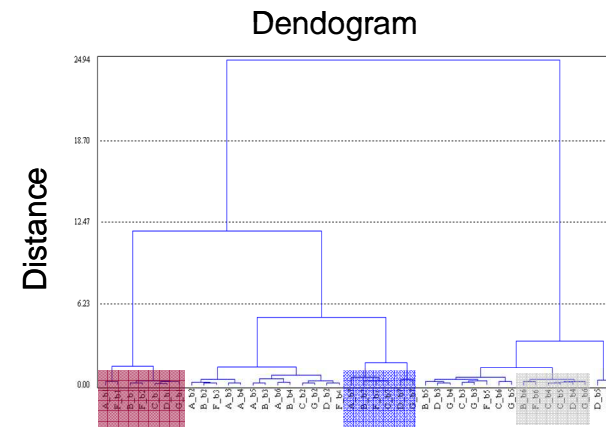
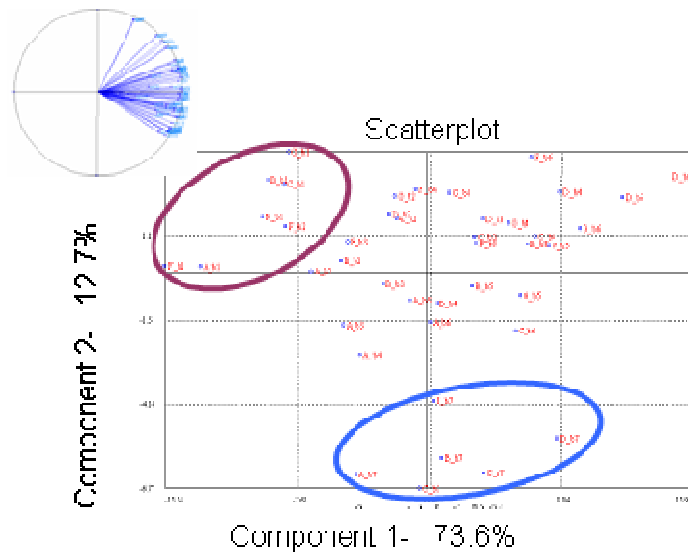
$7 < Tar < 10 \text{ mg/cig}$        $R^2 = 87.5\%$

- we plan to minimize the fragmentation pathway by working at lower ionization energy



# Data processing

- Individual spectra average by puff
- Principal Component Analysis and cluster analysis



# Screening results

## ■ cigarette paper study

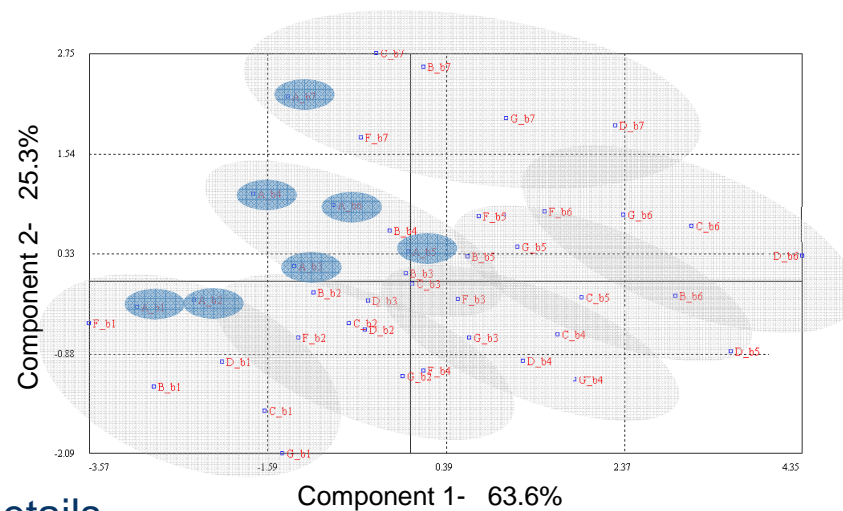
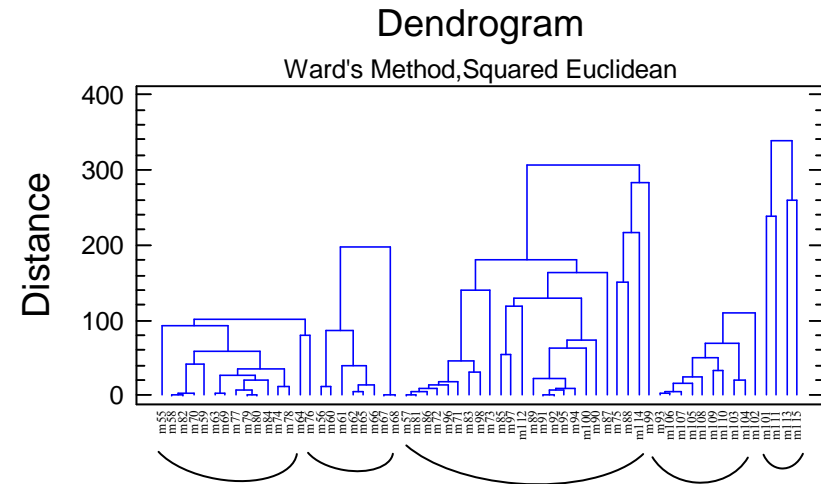
### → 6 prototype cigarettes

- Blend, weight, PD, Tar *under control*
- Different wrapper or filter paper.

### → Selection on m/z variables

- Clustering method: Ward's
- Distance Metric: Squared Euclidean
- Nber of clusters: 5.
- 7 first puffs

→ points out specific profile of product A which can be subsequently analyzed more in details



# Sum up & perspectives

## ■ We have achieved

- an easy-to-operate intuitive system
- an high-throughput method to perform routine qualification experiments

## ■ Next steps

- Continue data collection at lower IE.  
Continue data processing by applying CPA and Deconvolution methods
- Whole smoke study.

# Acknowledgements

- The French team
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