How chemometric tools can help for bidimensional chromatogram processing

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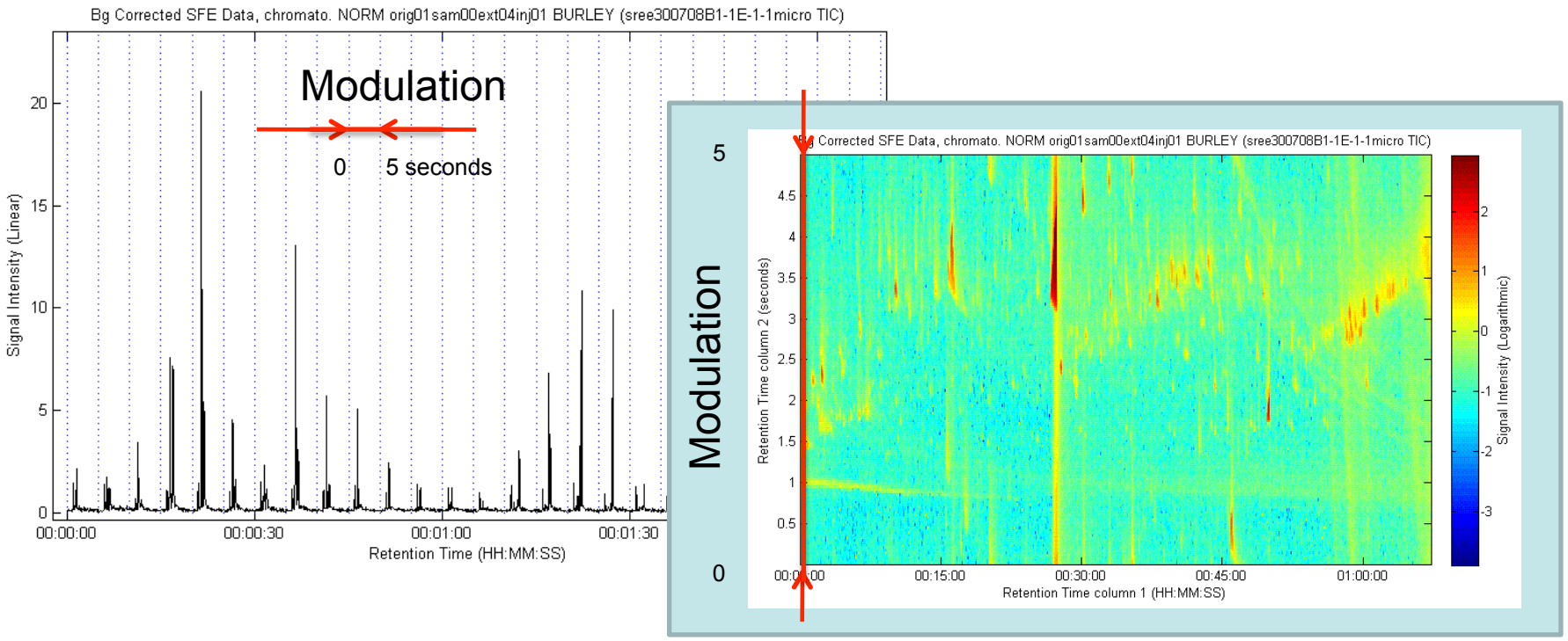
Analytics
Defis analytiques, du concept au système

îledeFrance

2D Data

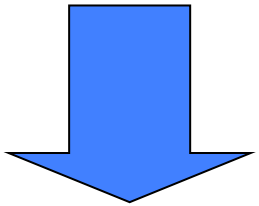
- Each chromatogram : > 100 000 pixels, several thousands of peaks



Need for helps to interprete!

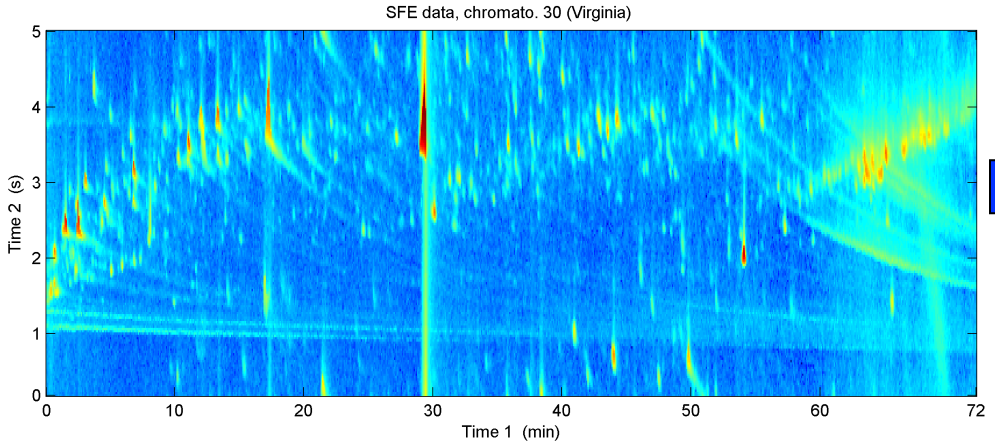
Data processing

- Data interpretation:
  - A simple transposition of 1D approaches is possible only in the case of target analysis of a limited number of compounds
  - For a global characterization of the sample: Visual exam of color plots?
  - No general solution available :
    (specific solutions in some domains)



Need to develop a strategy for the automatic comparison of chromatograms and the identification of discriminant compounds

General strategy



Each pixel is considered as a response with a given intensity

Global comparison carried out using multivariate analysis tools like PCA

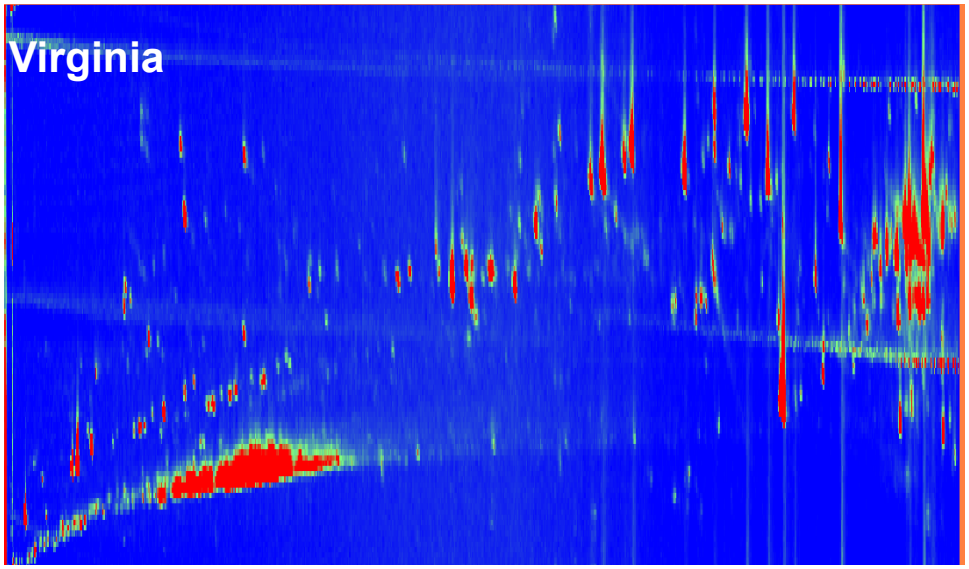
Discrimination of the samples

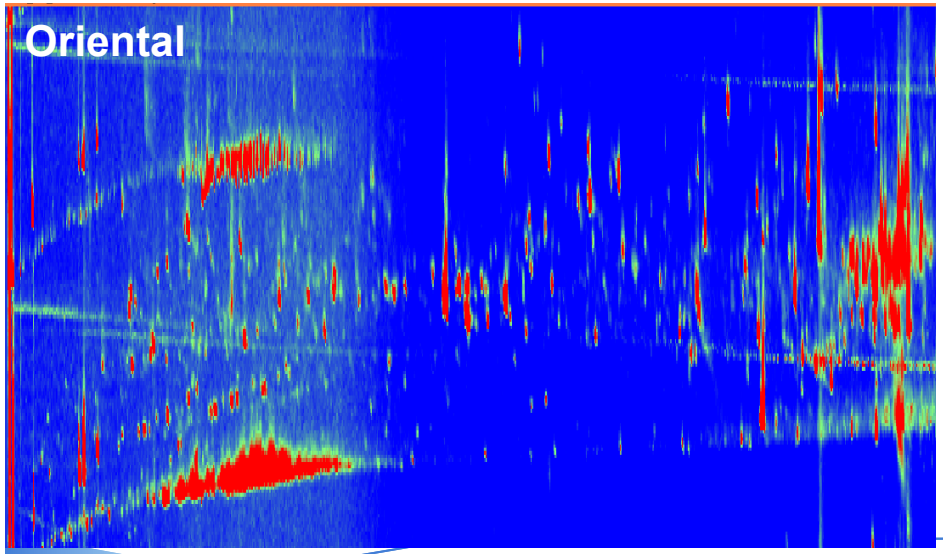
Identification of the differences

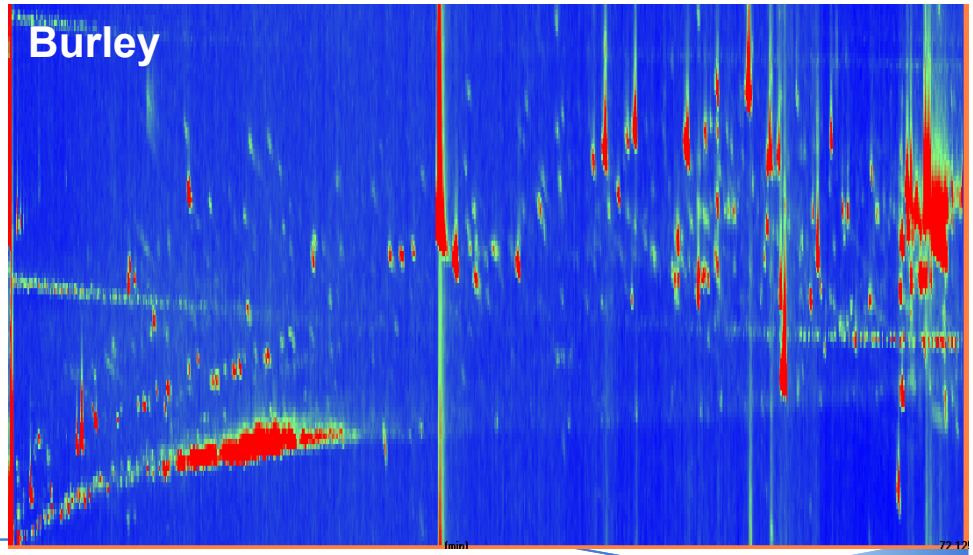
Example of application

Conditions :

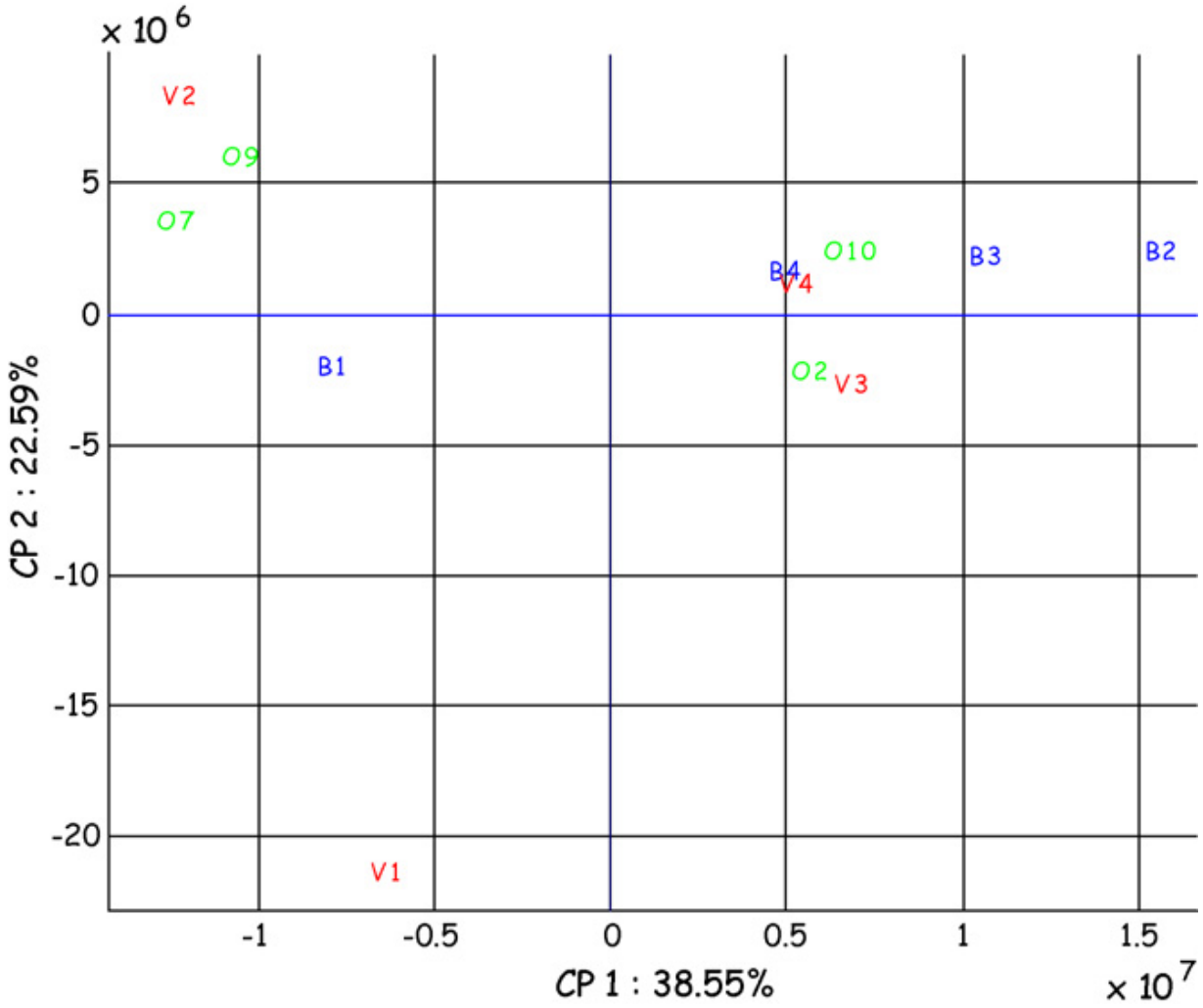
- 12 tobacco extracts (≠ smokes) analyzed by GCxGC
- 3 types of tobacco: Burley, Virginia and Oriental
- 4 samples of ≠ origin per tobacco type







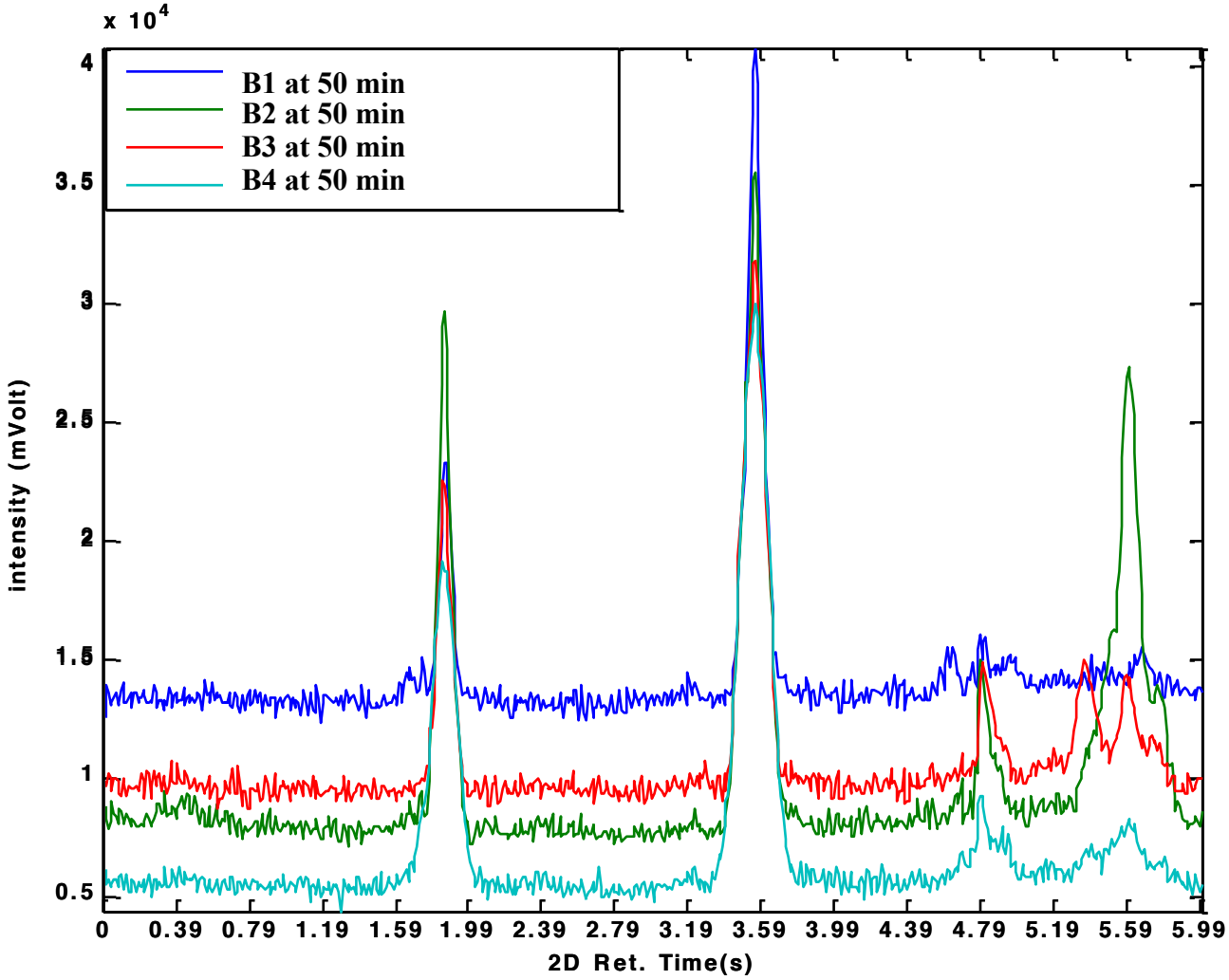
PCA results



No discrimination: necessity of a data pretreatment

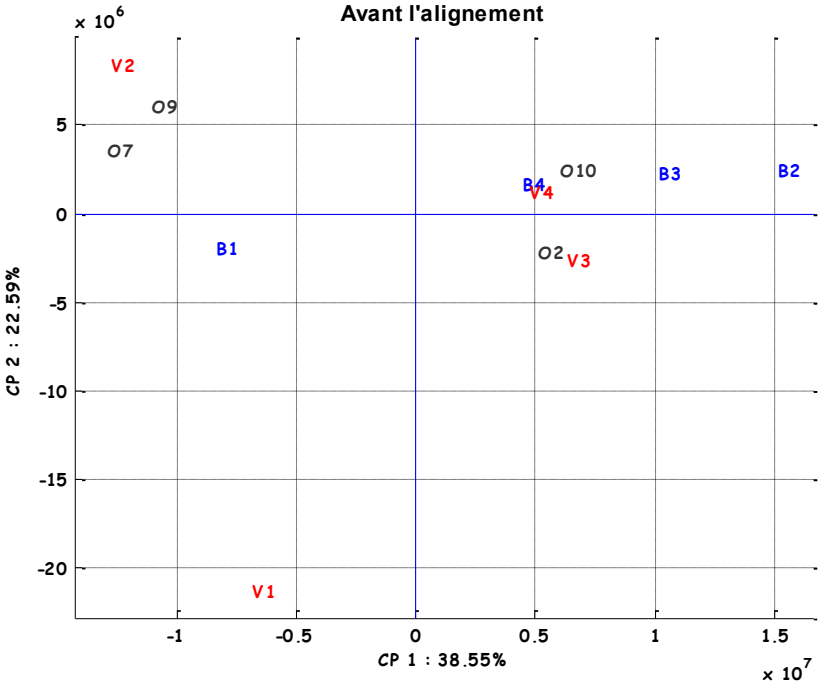
Cause

Use of Dynamic Time Warping (DTW)

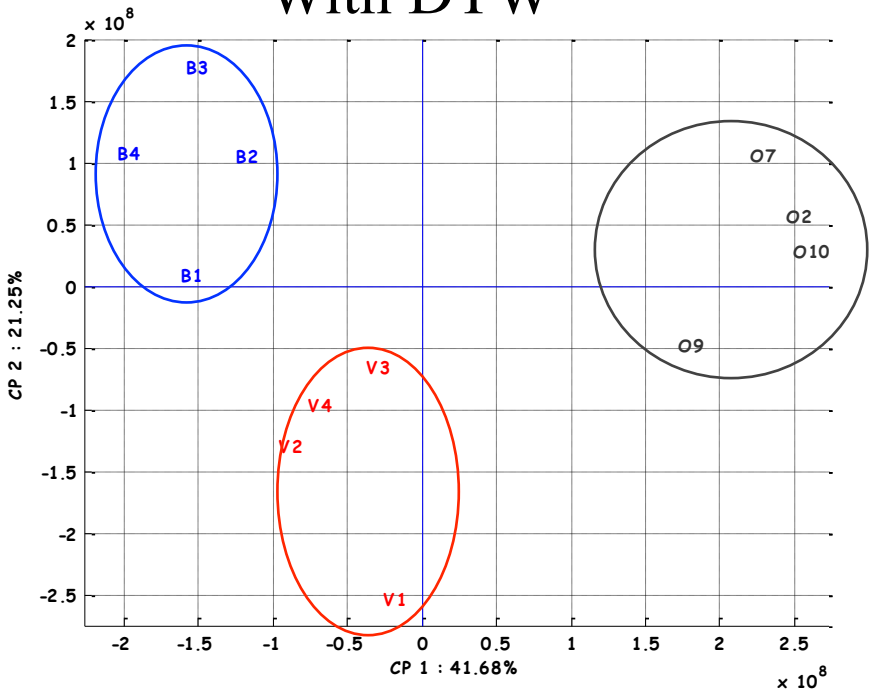


Impact on classifications

Without DTW



With DTW

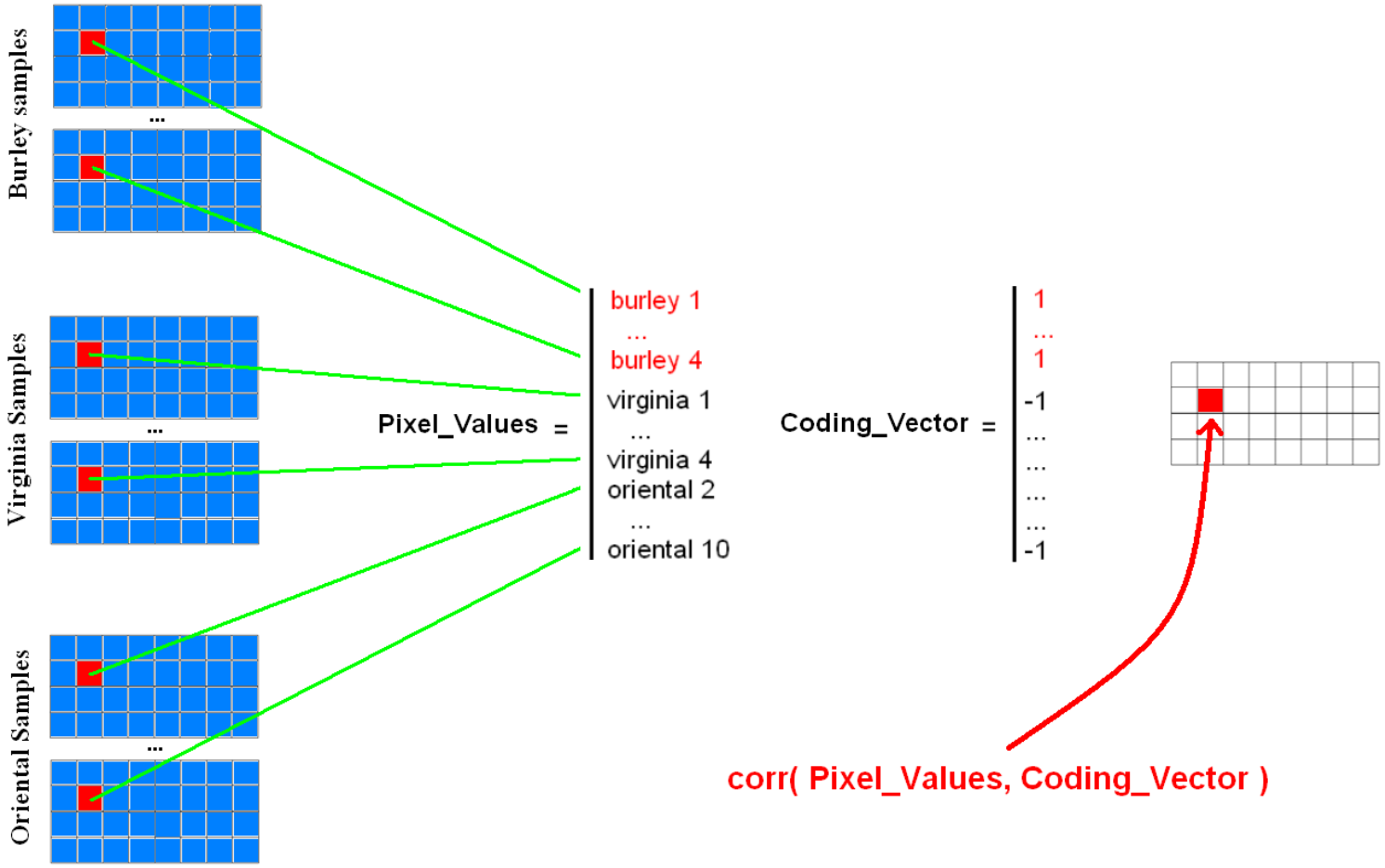


J. Vial, H. Noçairi, P. Sassiat, S. Mallipattu, G. Cognon, D. Thiébaut, B. Teilllet, D. N. Rutledge, J. Chromatogr. A, ***2009,*** *1216, 2866-2872.*

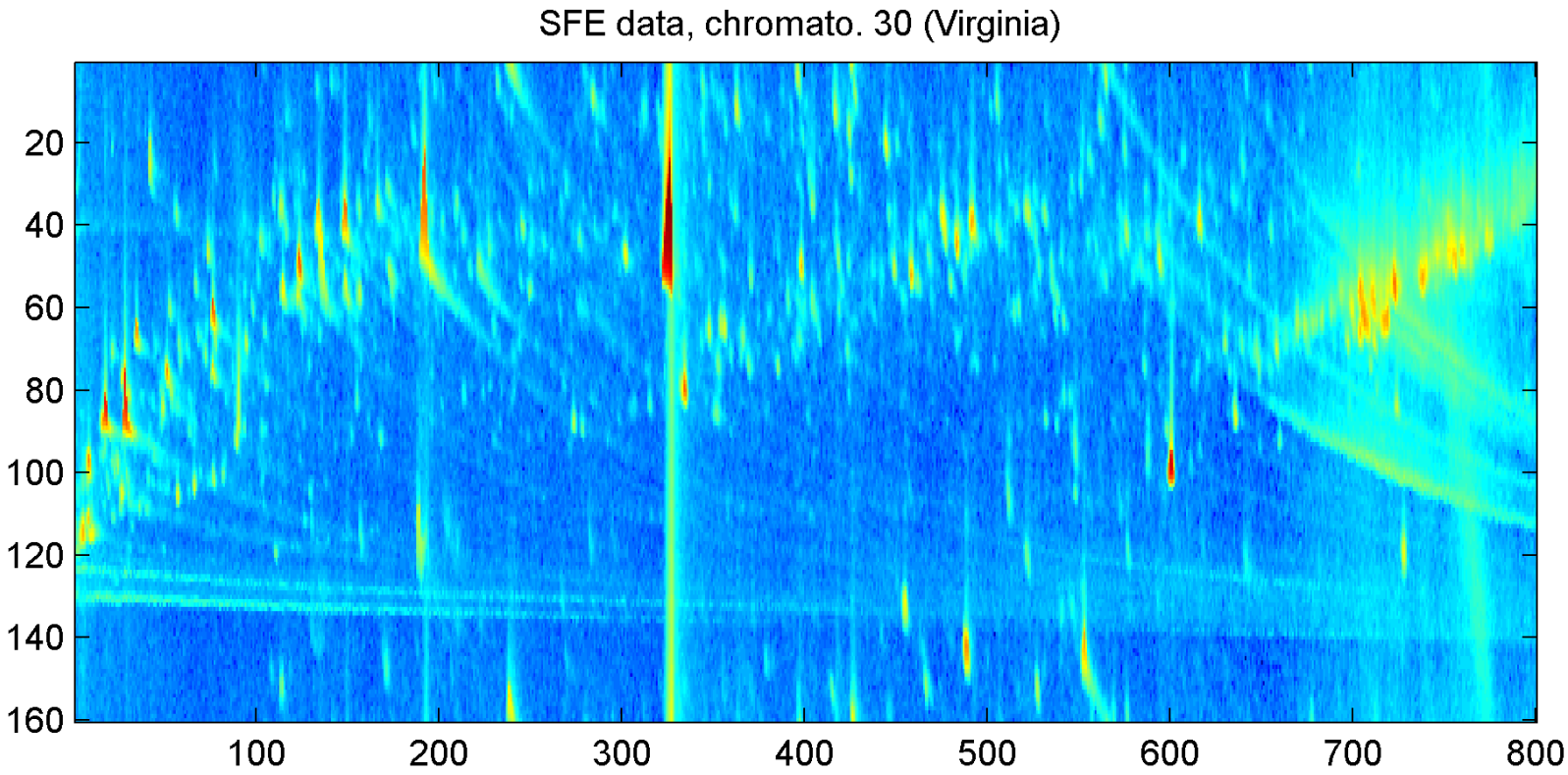
Search for markers

Discriminant pixels

- Comparison of samples from a tobacco type to all other samples

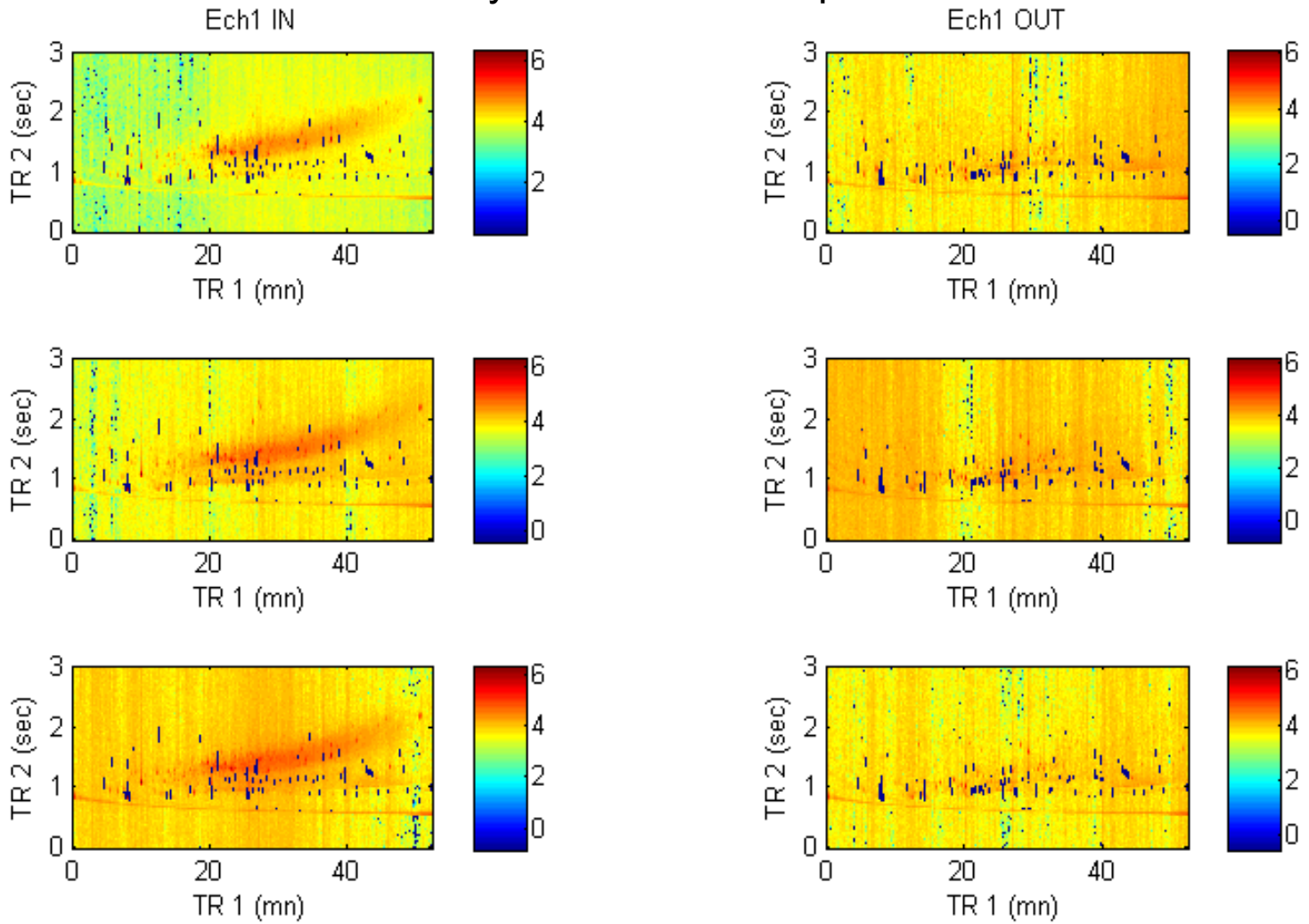


Results: SFE data



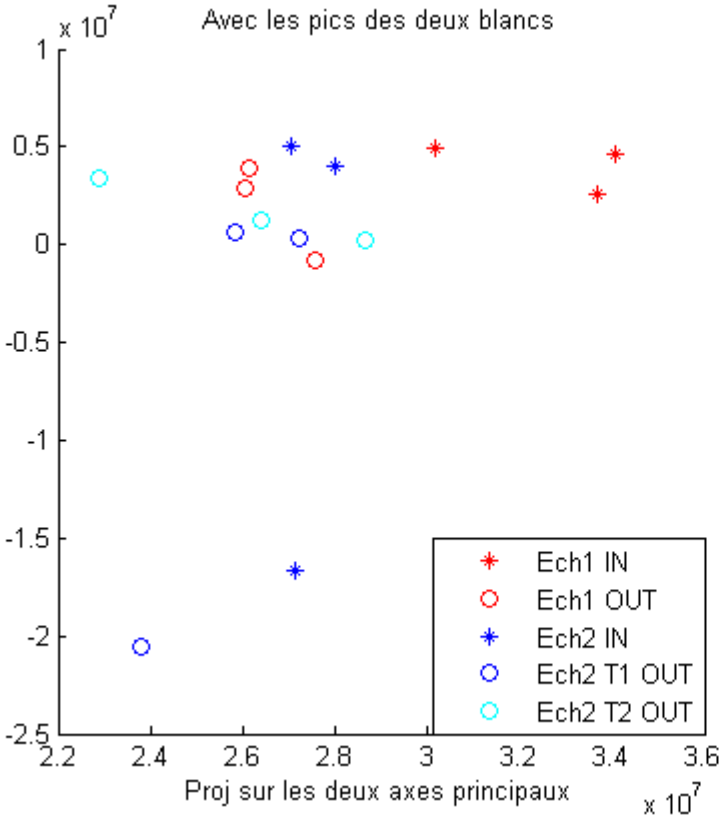
Environmental application

SBSE-GCxGC-TOF/MS analysis of water samples before and after treatments.

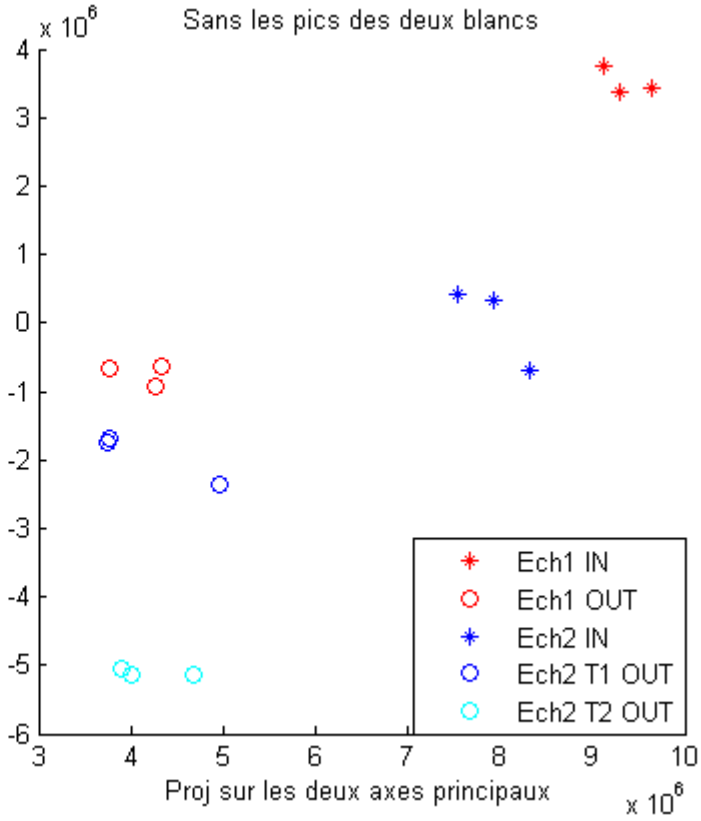


PCA

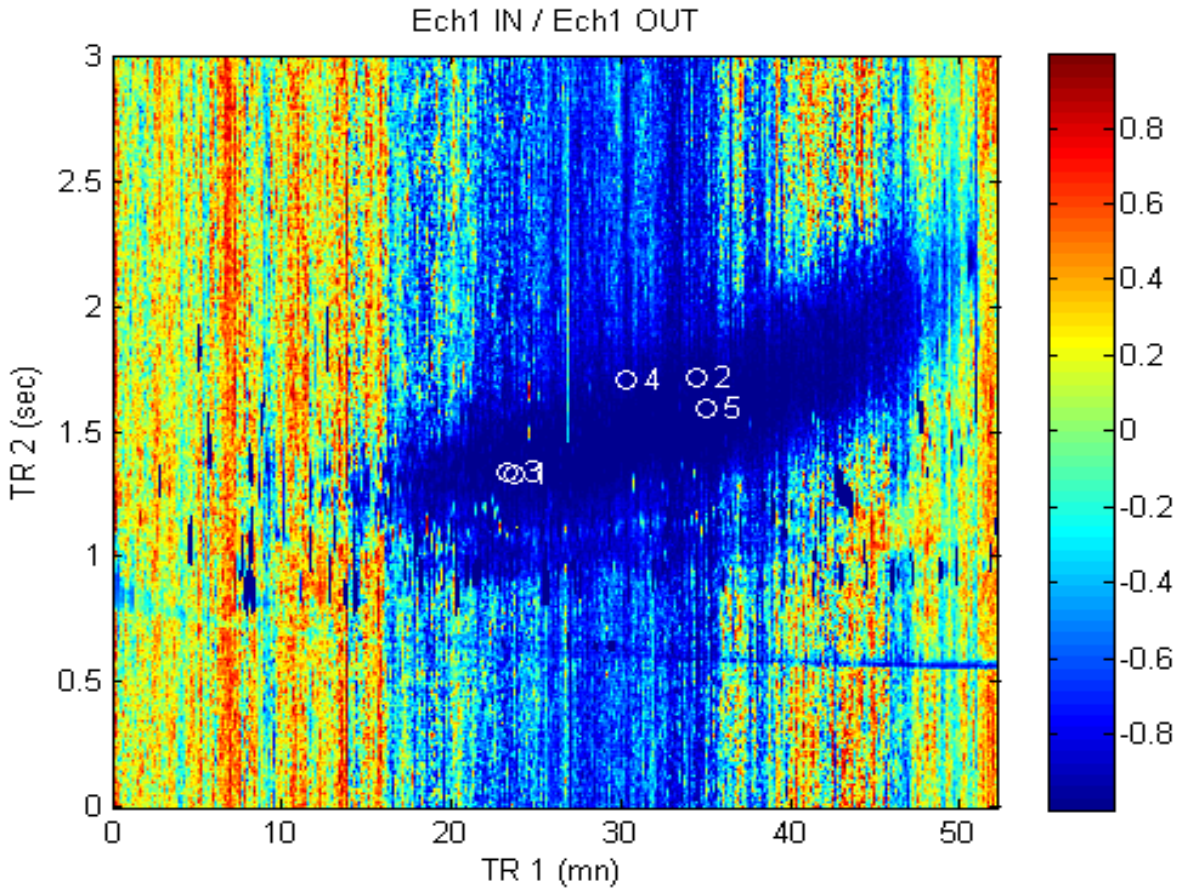
With peaks present in the blank



After removal of the peaks present in the blank

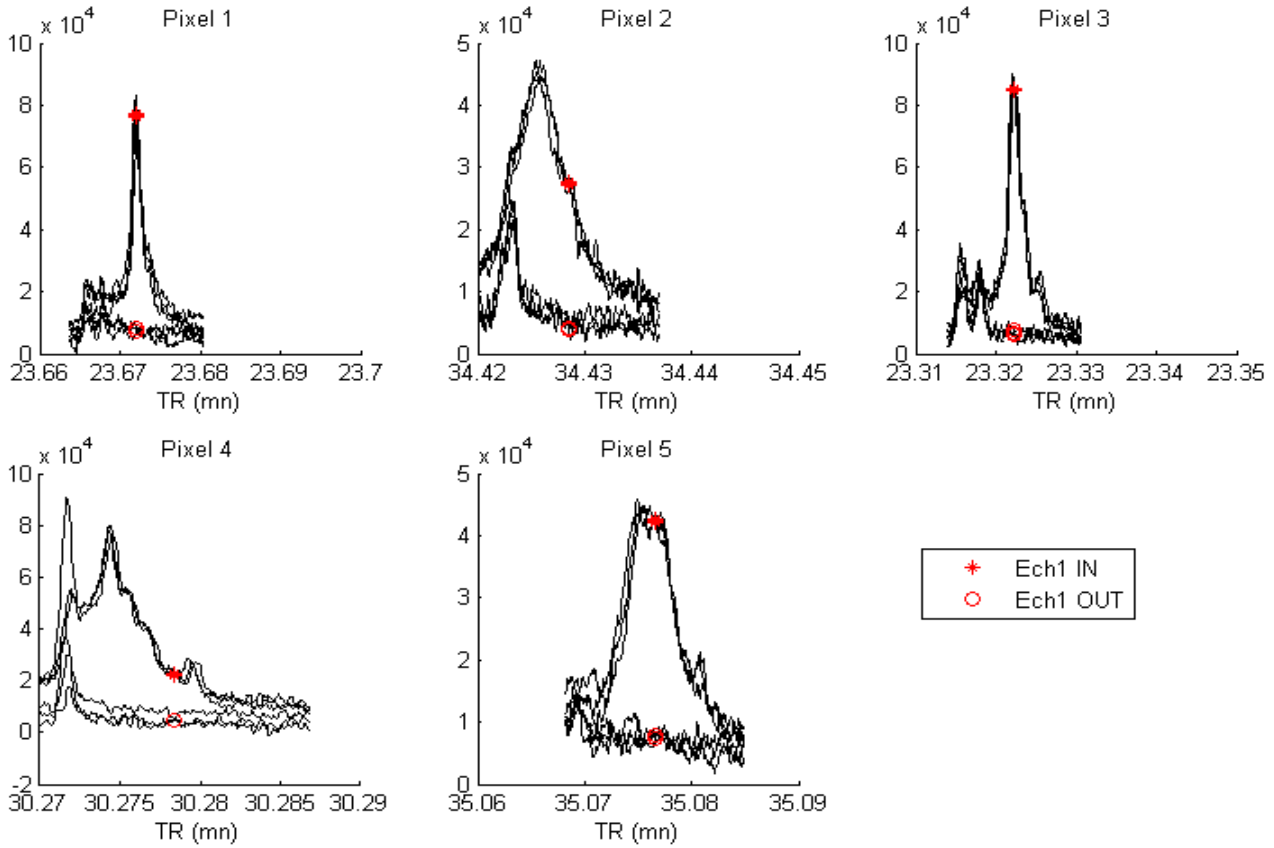


Correlation maps Ech1 IN vs OUT



Discrimination *Ech1 IN* / *Ech1 OUT*. Pixels correlation of which is close to -1 (dark blue) are those intensity is lower after treatment

Chromatographic illustration



5 discriminant pixels for *Ech1 IN* (*) vs *Ech1 OUT* (o)

Conclusion

- Proposal of strategies based on chemometric tools:
  - Data preprocessing (BG correction, normalization)
  - Time alignment
  - PCA (samples comparison) : type discrimination
  - Class map
  - Discriminant pixels ➔ Discriminant 2D peaks

Interactive

Applications

- Discrimination of tobacco extracts with identification of type markers
- Determination of water treatment efficiency (trace analysis)

↳ New kind of samples, improvements of the tools


Thank you for your attention!
Questions?