

# Fingerprints of tobacco smoke precursors by comprehensive GCxGC

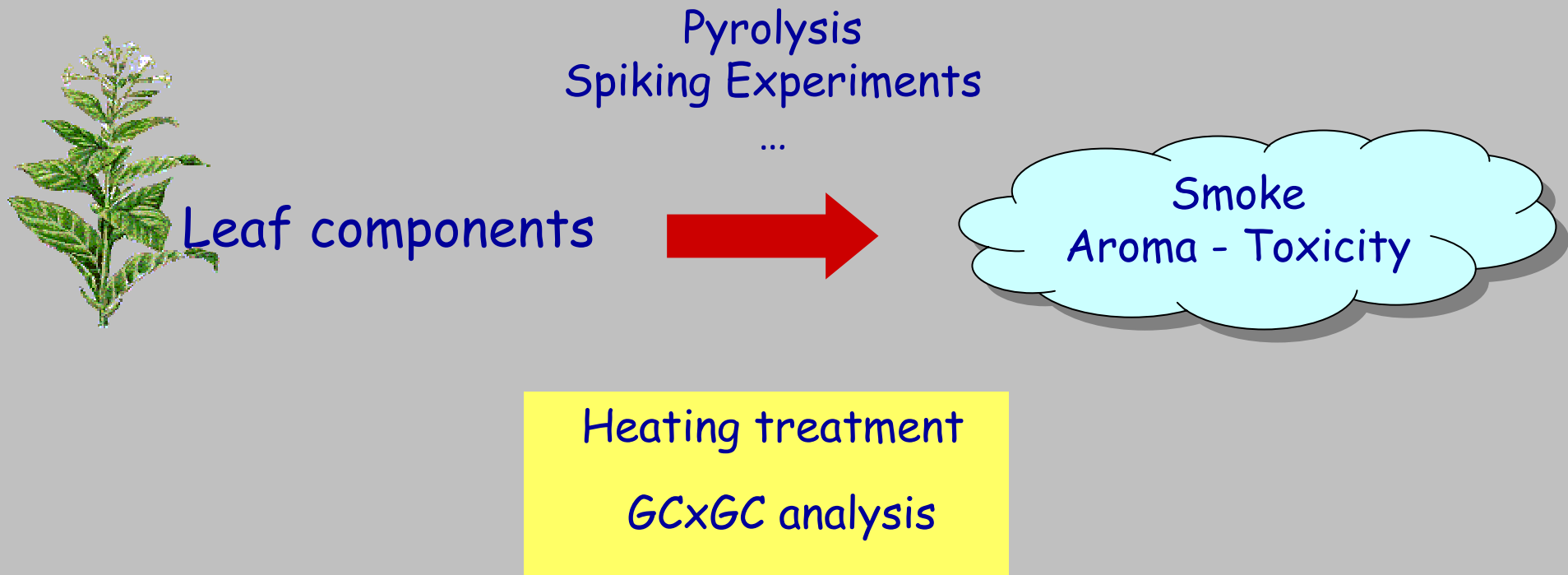
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Altadis Research Center - France

50th Coresta Congress - Paris



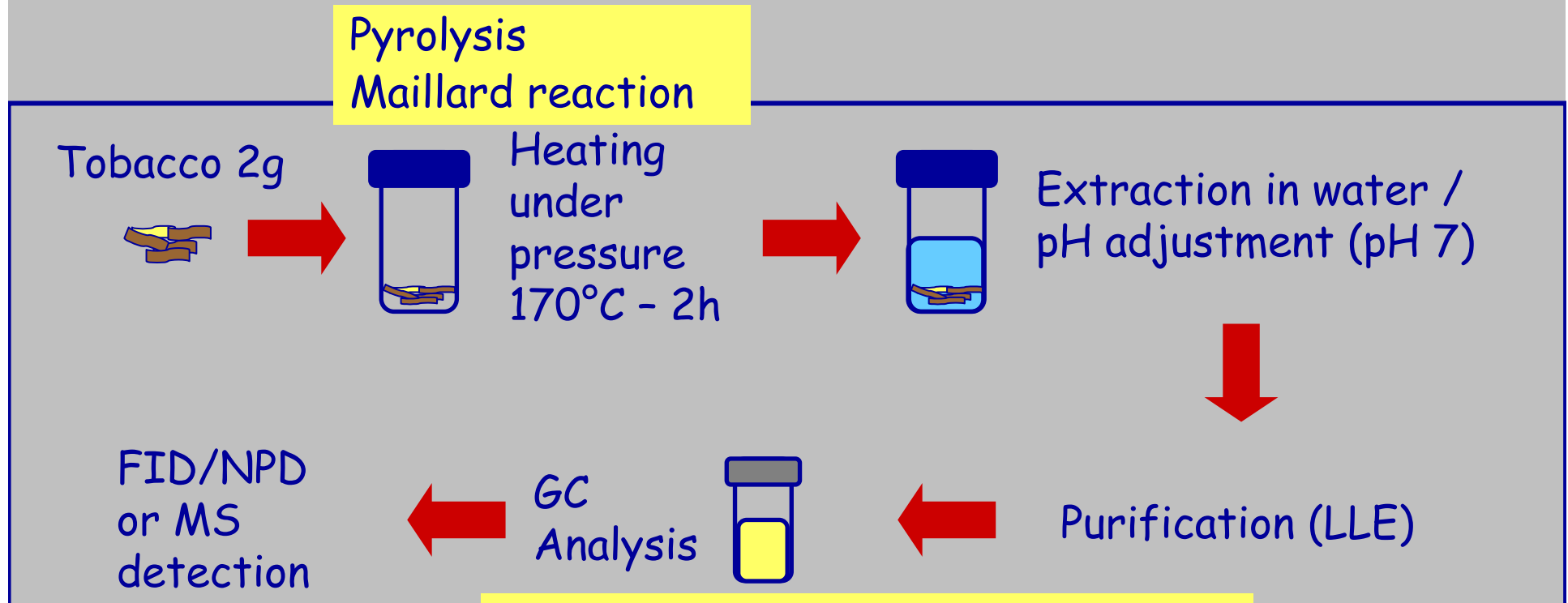
# Introduction



## ✕ Plan

- Tobacco heating treatment
- GCxGC principle & advantages
- Optimisation of GCxGC for heated tobacco samples
- Applications

# Sample preparation

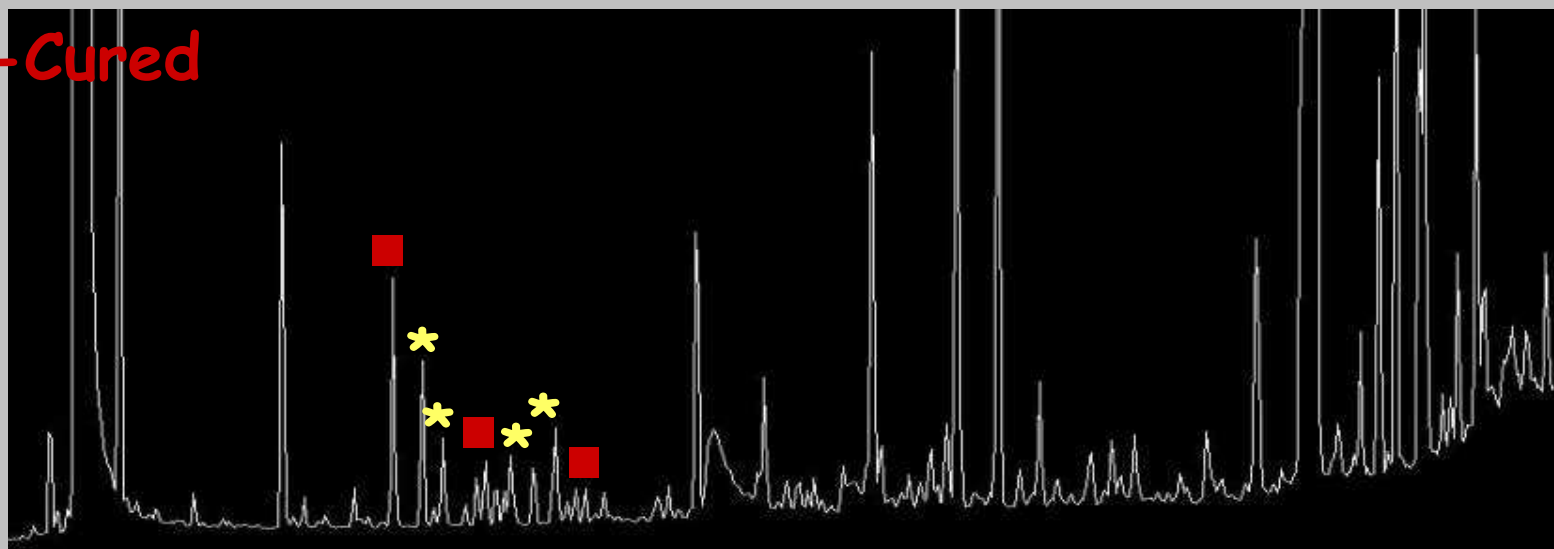


lactones, ketones, cyclopentanes,  
short chain carboxylic acids,  
furfurals, furans, furanones,  
pyrroles, pyridines and pyrazines

✘ Image of the carbohydrates / nitrogenous balance during combustion

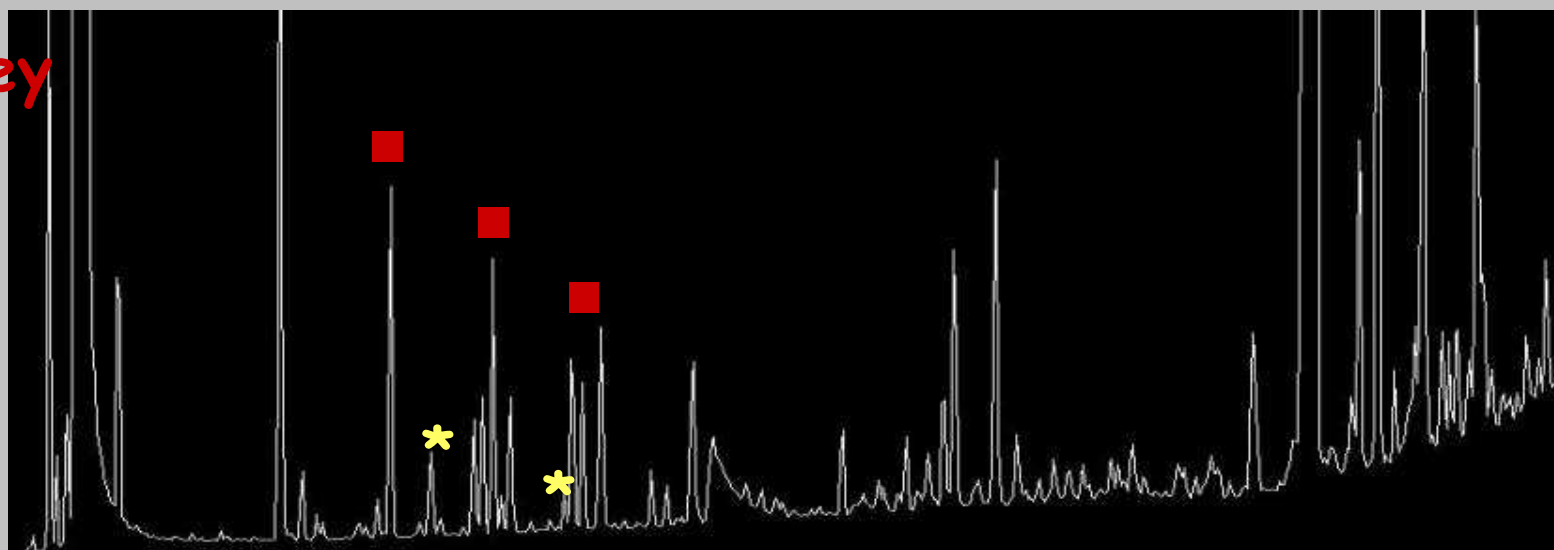
# Sample analysis - Limitation of GC analysis for profiles comparison

Flue-Cured

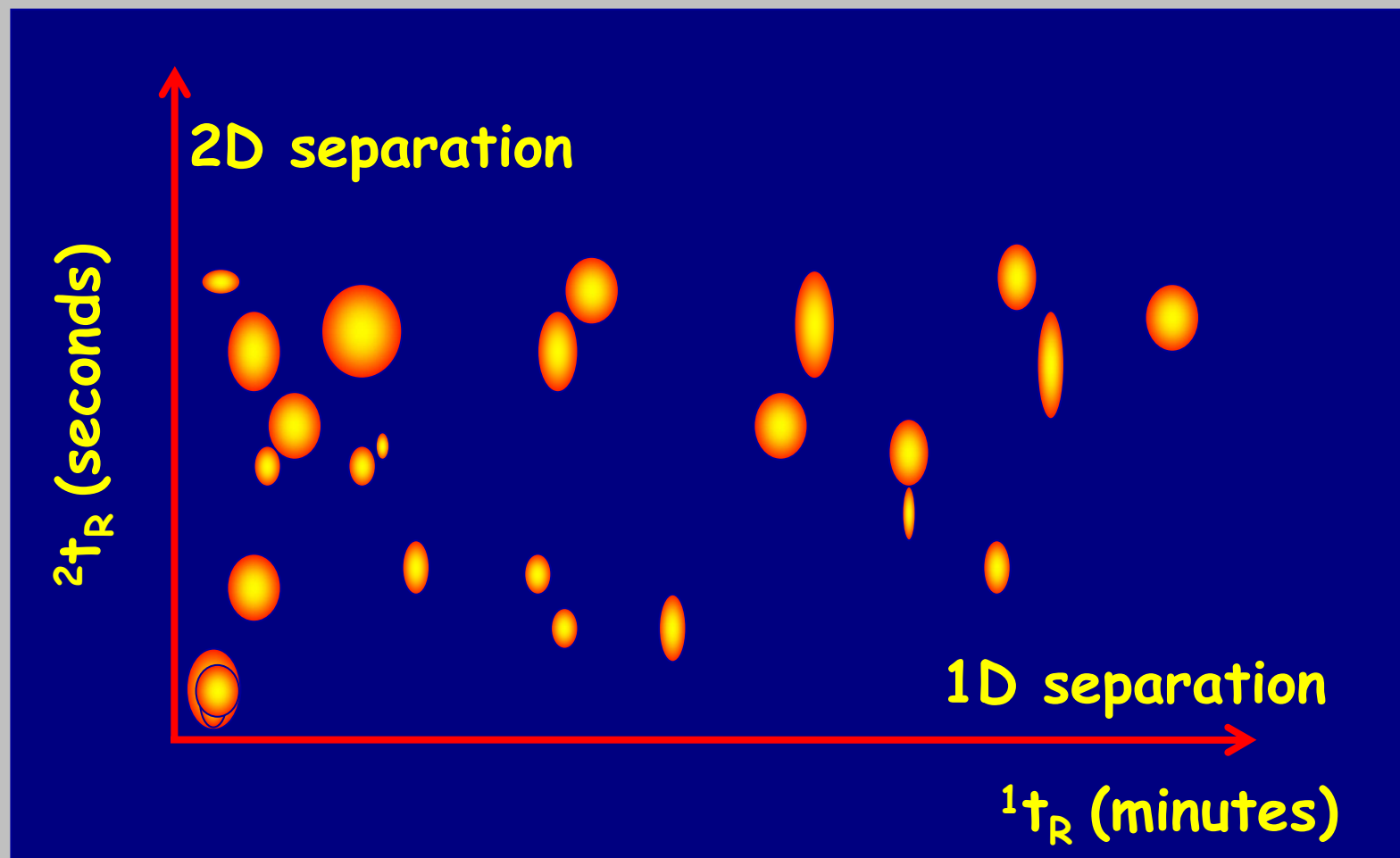


■ pyrazines  
\* ketones

Burley



# Advantages of comprehensive GCxGC



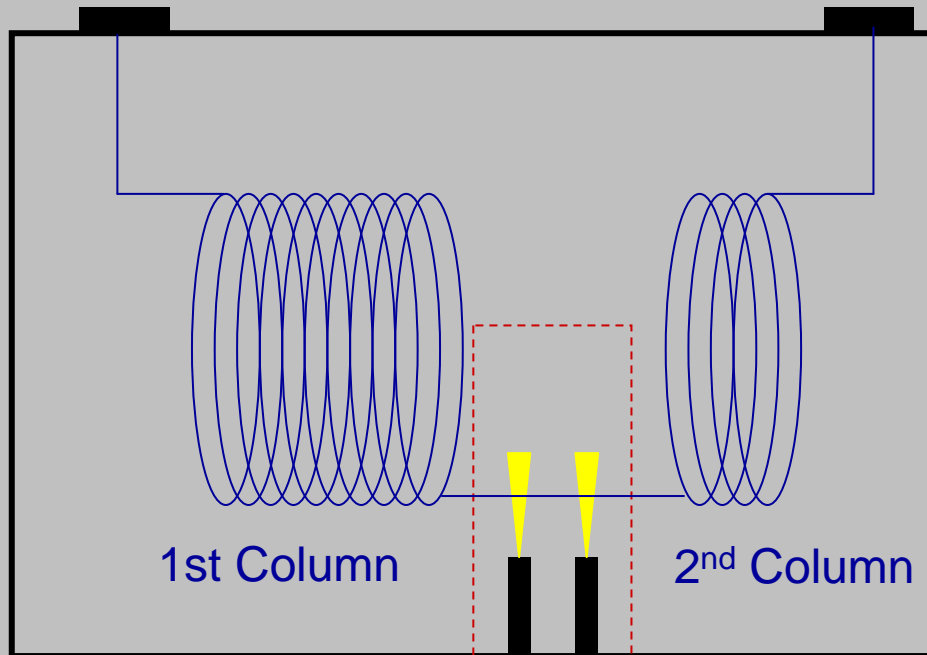
- ✘ Improved separation power
- ✘ Organized chromatograms

# GCxGC system

Trace GCxGC Ultra ThermoElectron

Split/Splitless  
Injection Syst

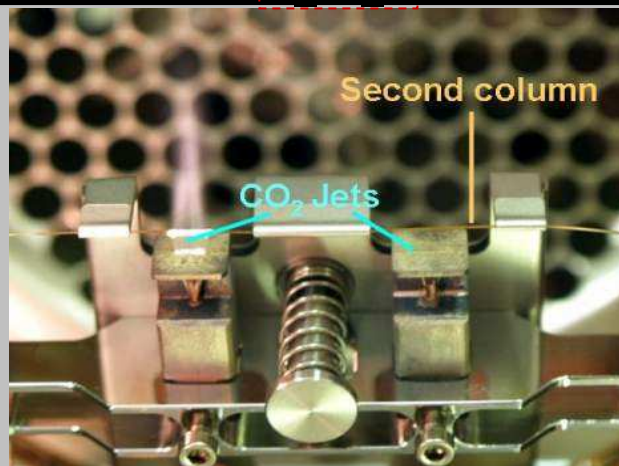
Fast FID  
Detector



1st Column

2nd Column

Cryogenic  
modulator  
Double CO<sub>2</sub>  
jets



①

Cryogenic modulation

CO<sub>2</sub>

1st column

2nd column

②

Cryogenic modulation

CO<sub>2</sub>

1st column

2nd column

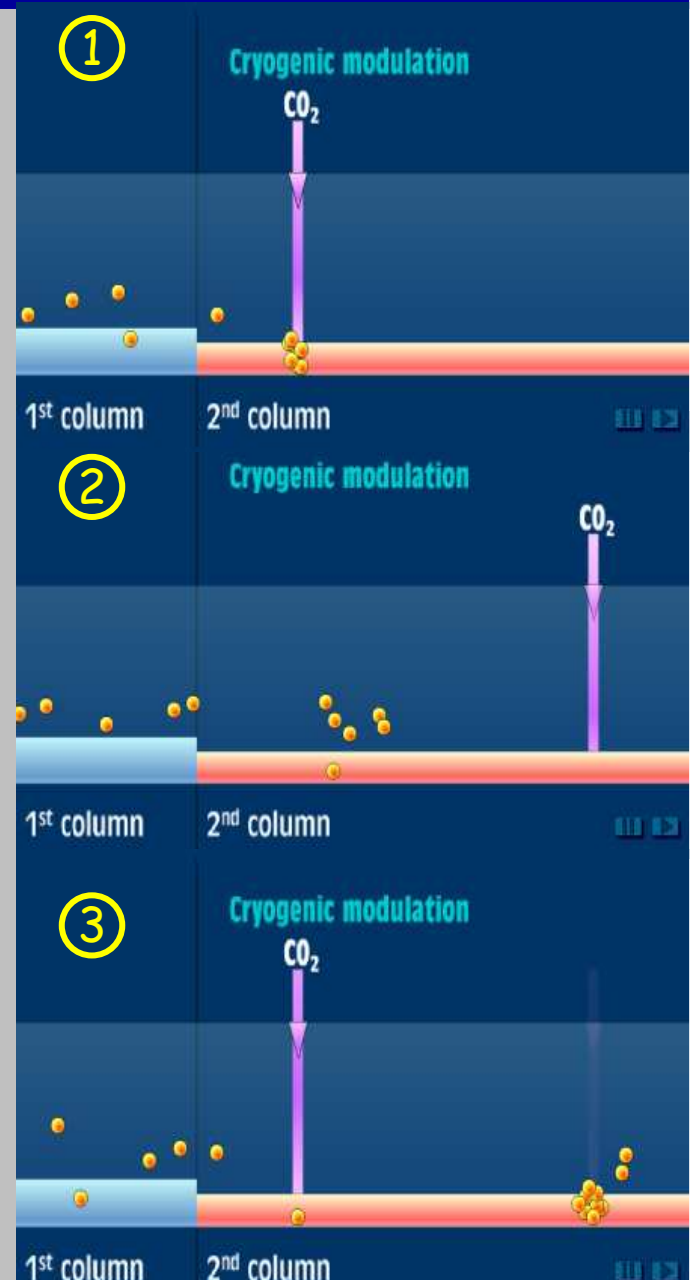
③

Cryogenic modulation

CO<sub>2</sub>

1st column

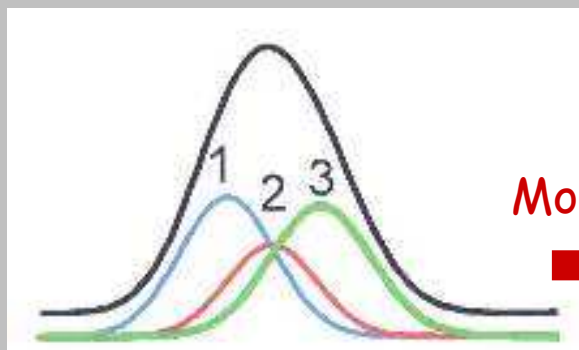
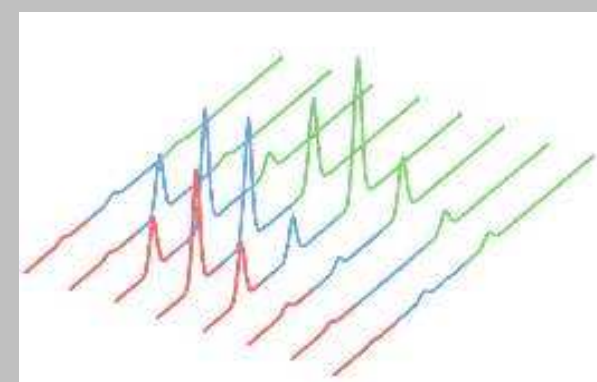
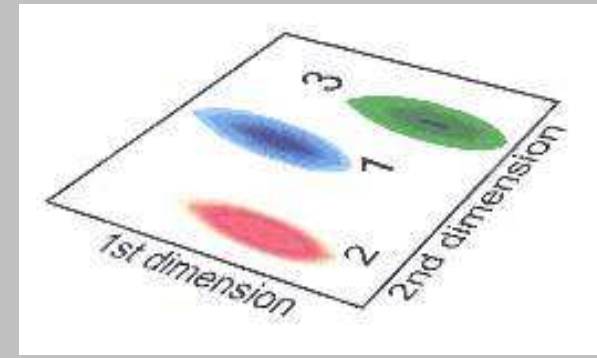
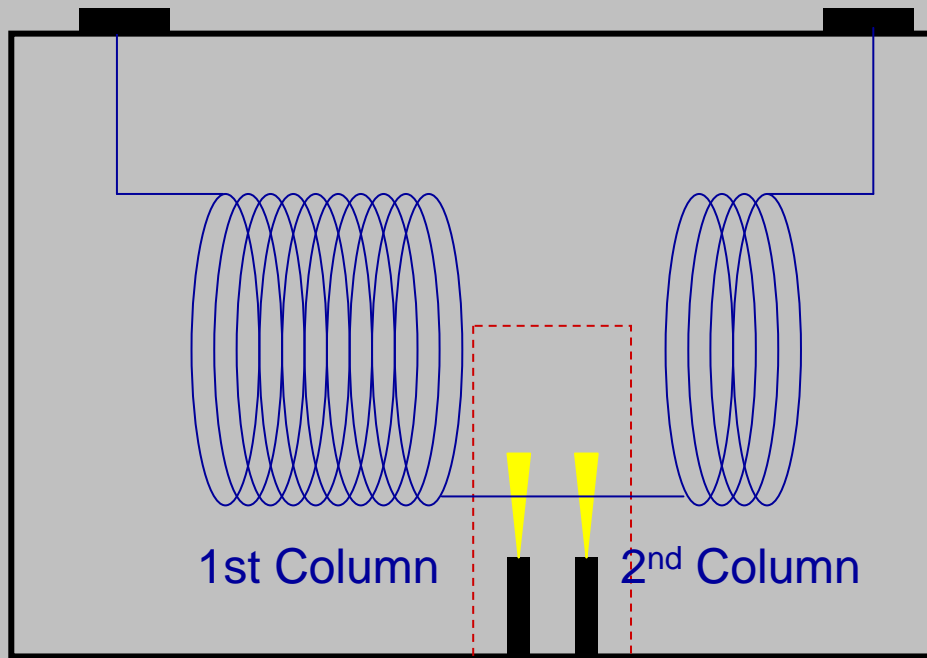
2nd column



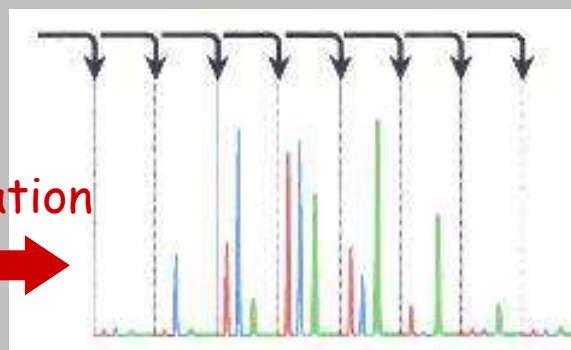
# GCxGC system

Trace GCxGC Ultra ThermoElectron

Split/Splitless Injection Syst      Cryogenic modulator  
Double CO<sub>2</sub> jets      Fast FID Detector



Modulation



Data transformation



# Optimisation of the separation

## ✧ Parameters

- Columns phases : apolar/polar vs polar/apolar
- Columns lengths
- Temperature program

## ✧ Samples

- Standard solution of model solutes
- Heated Tobacco extracts

furanones  
furans  
furaldehydes  
pyrazines  
pyridines  
pyrrolidinones  
pyrroles

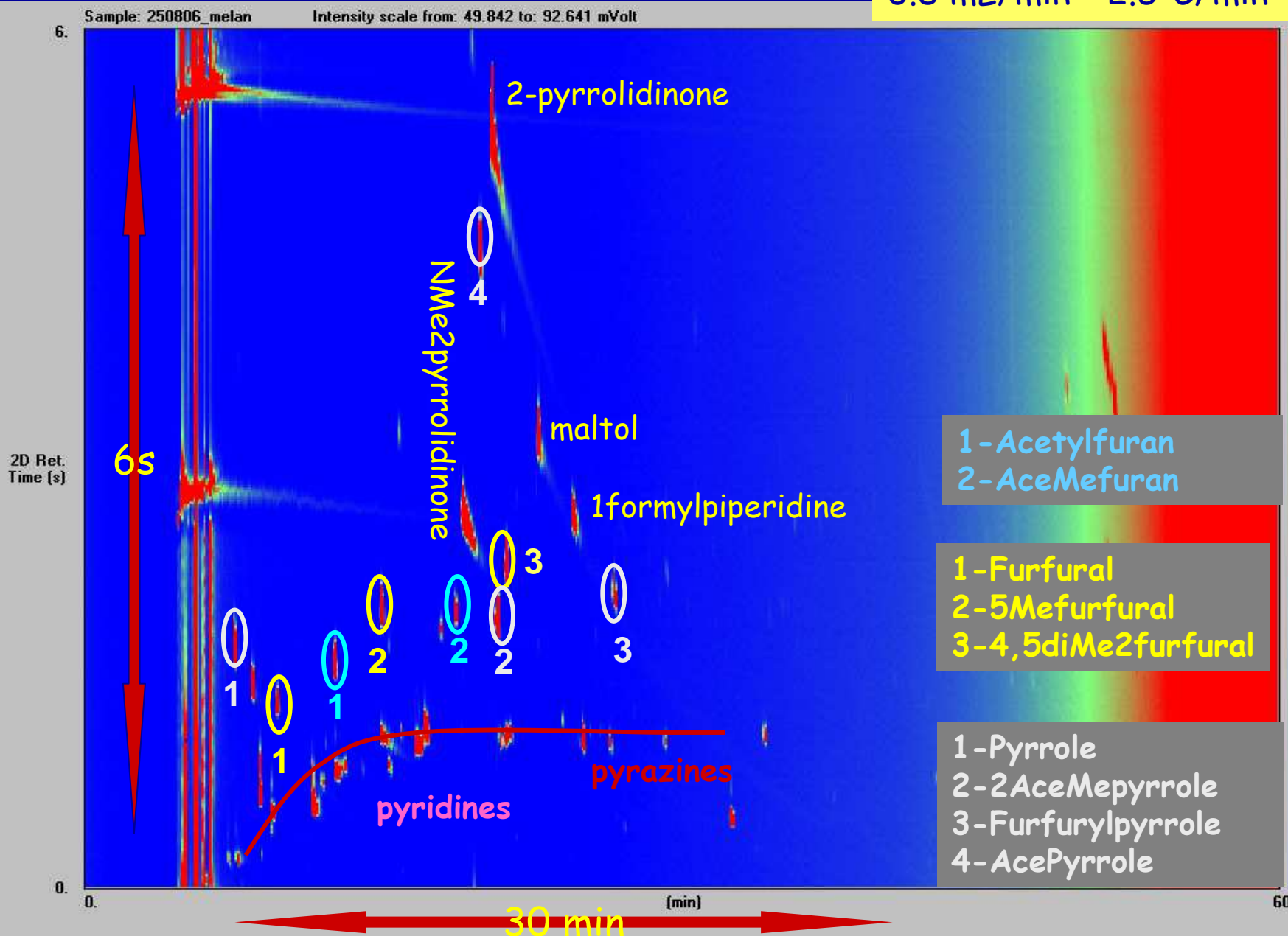
## ✧ Objective

- Good distribution of the compounds over the 2D plane
- Separation of the main families of compounds
- Best discrimination between tobacco types



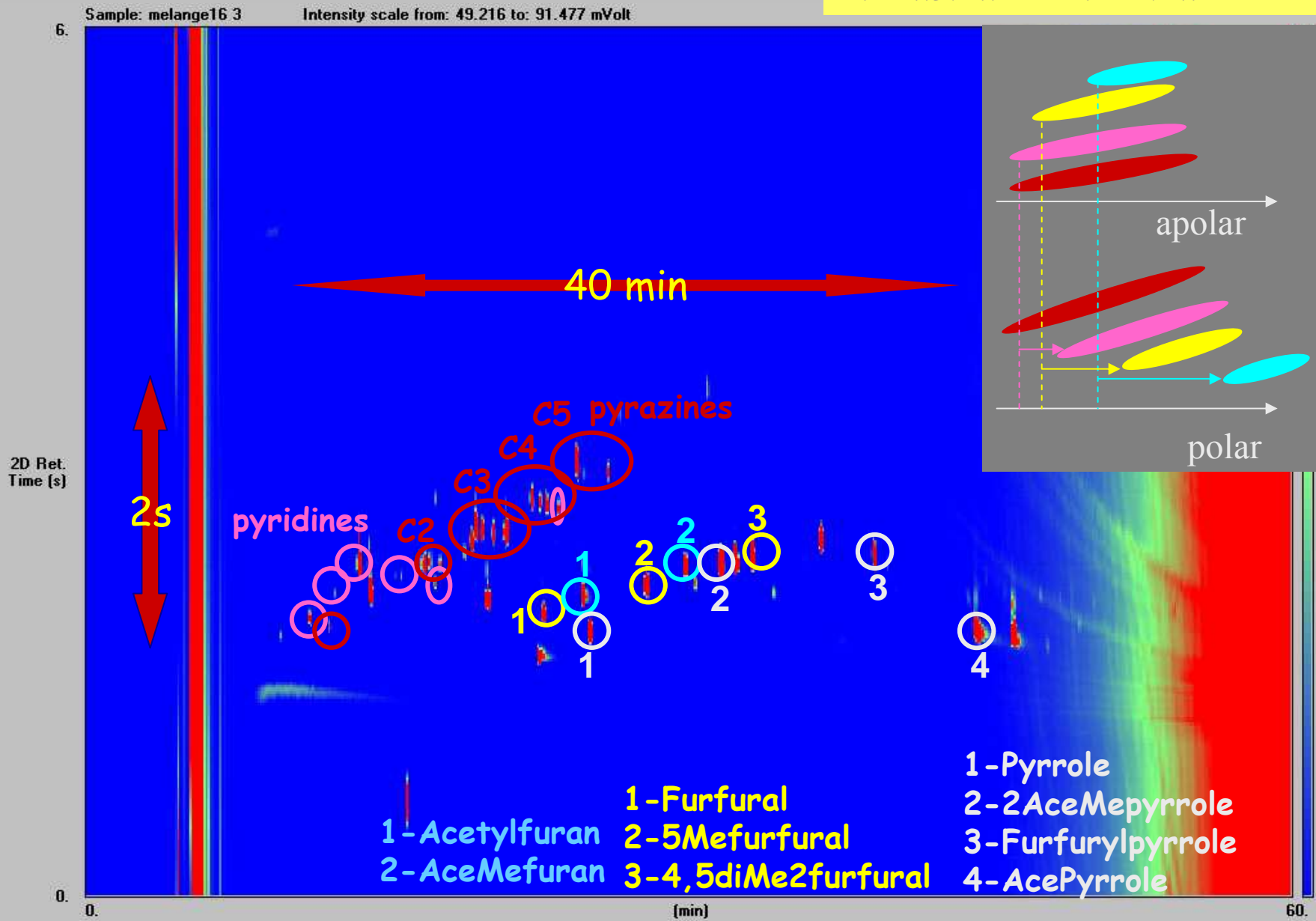
# Normal Phase GCxGC

RTX5 30m x 0.25mm x 0.25 μm  
RTX1701 1m x 0.1 mm x 0.1 μm  
0.8 mL/min - 2.5°C/min



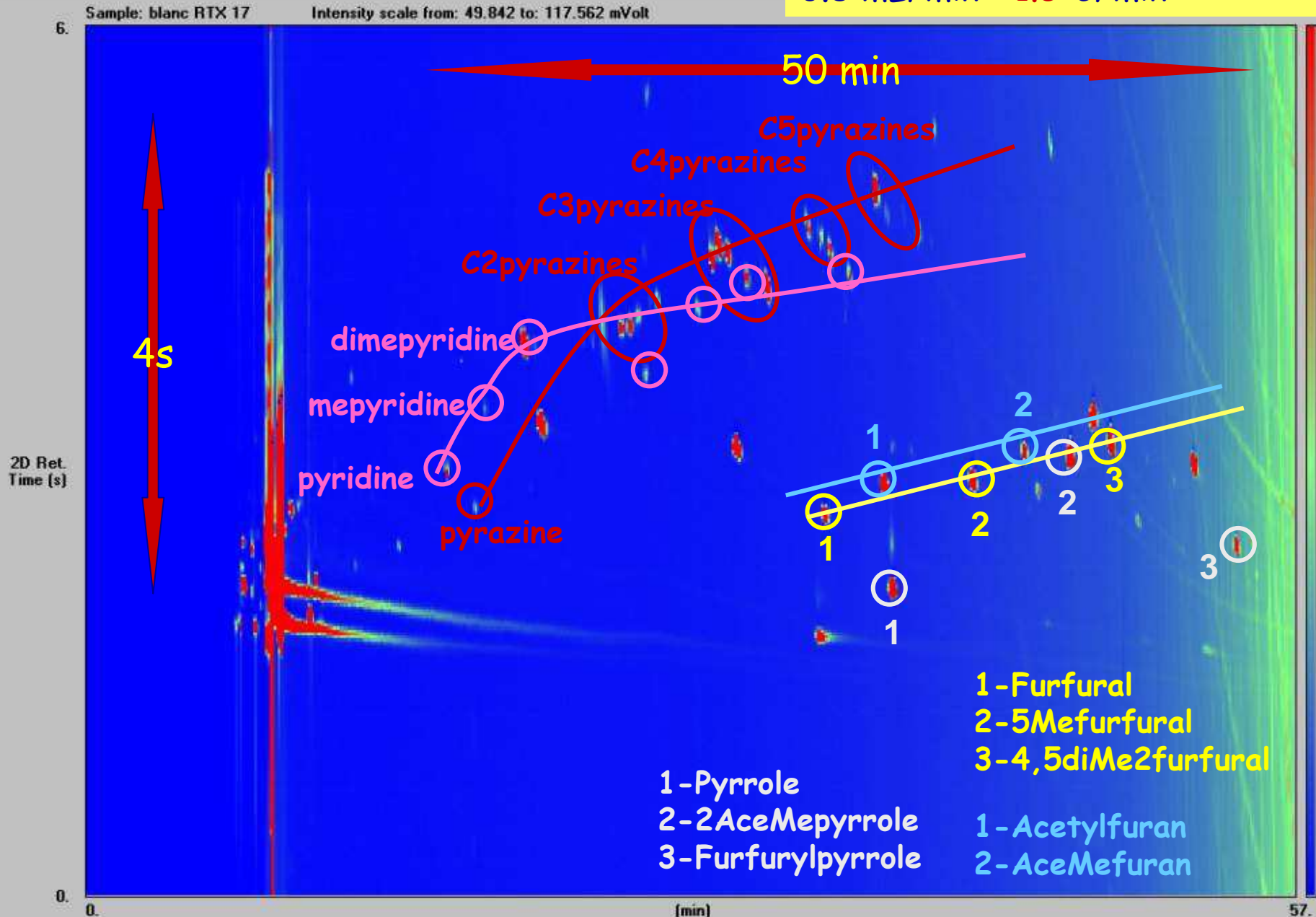
# Reverse Phase GCxGC

Solgelwax 30m x 0.25mm x 0.25 μm  
RTX1701 1m x 0.1 mm x 0.1 μm  
0.8 mL/min - 2.5°C/min

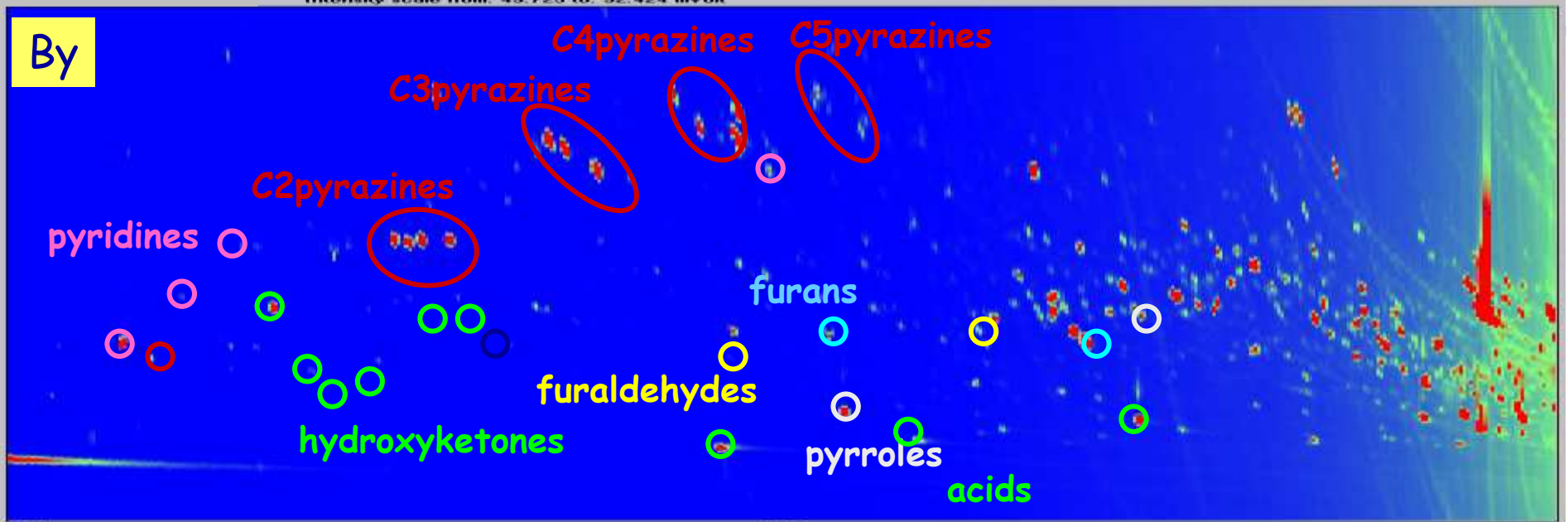


# Column Length/ Temperature program

Solgelwax 30mx0.25mmx0.25 $\mu$ m  
 RTX1701 2mx0.1 mmx0.1  $\mu$ m  
 0.8 mL/min - 1.5 $^{\circ}$ C/min



# Tobacco comparison



# 1D Profiles

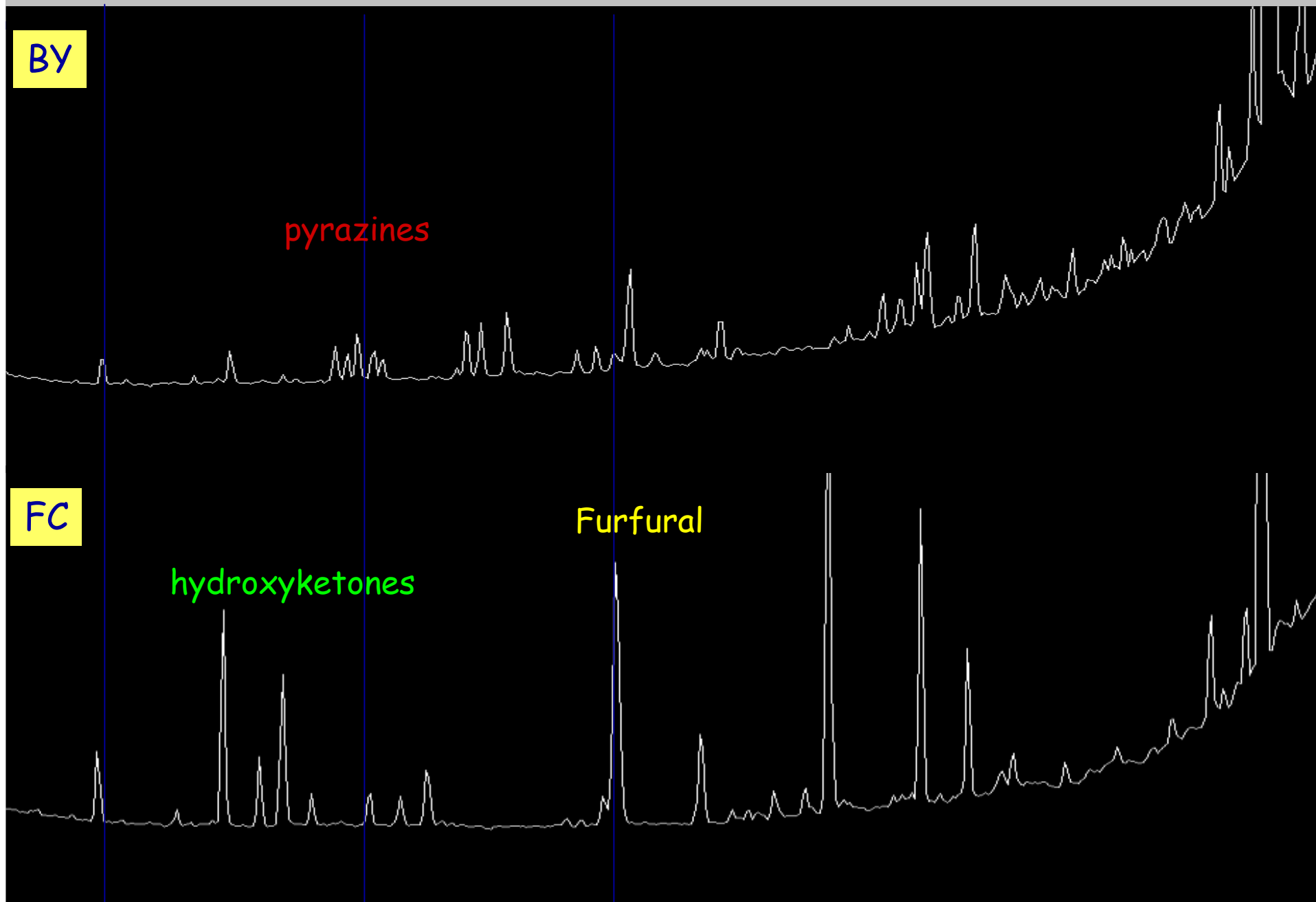
BY

pyrazines

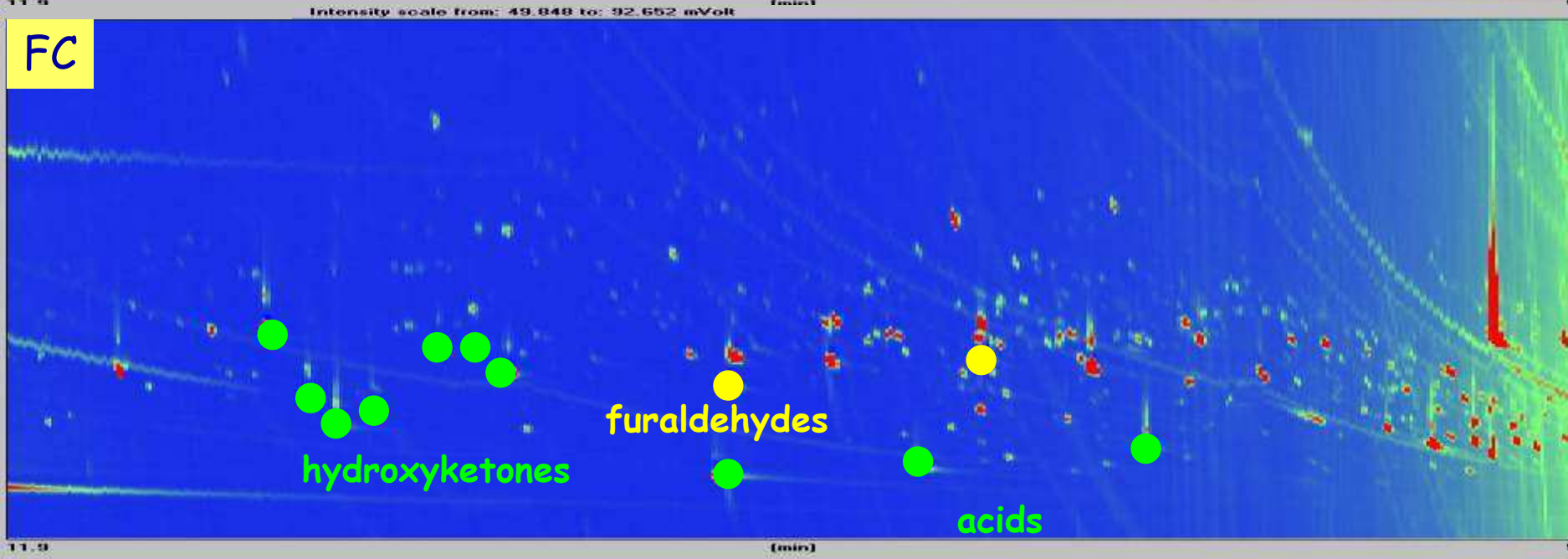
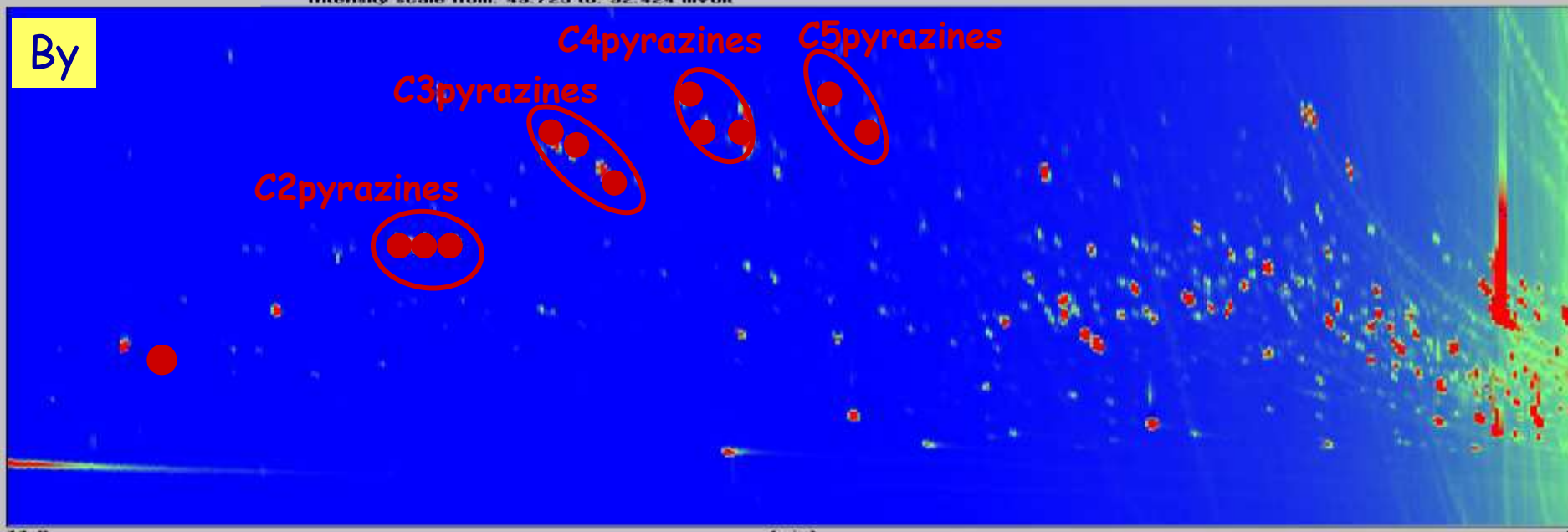
FC

hydroxyketones

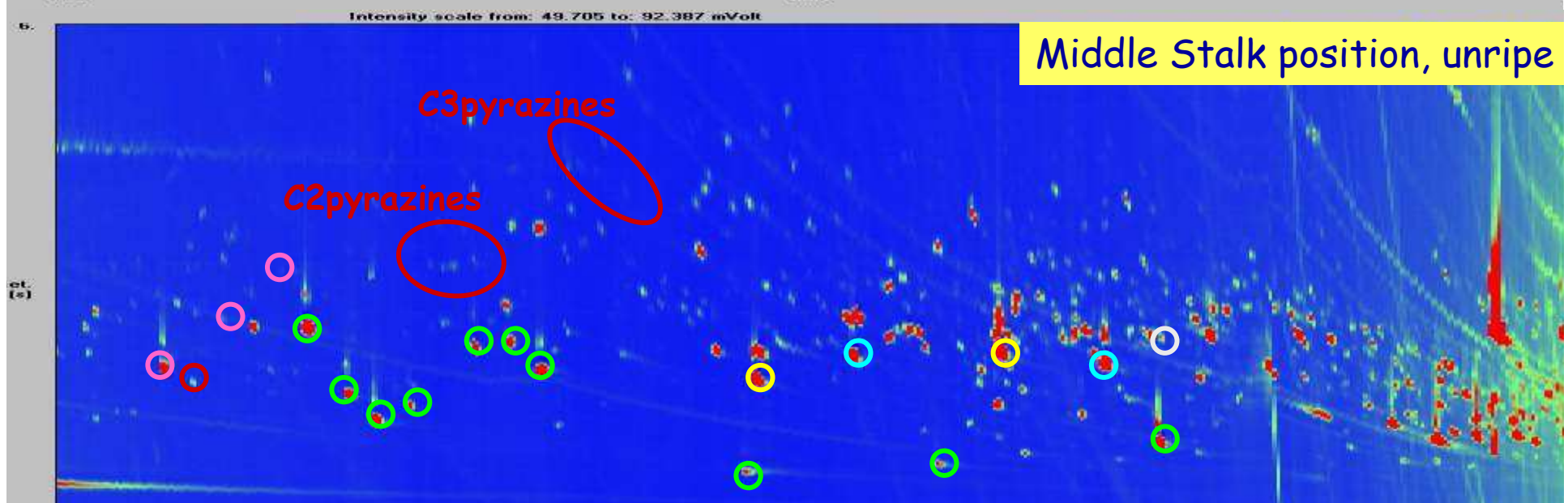
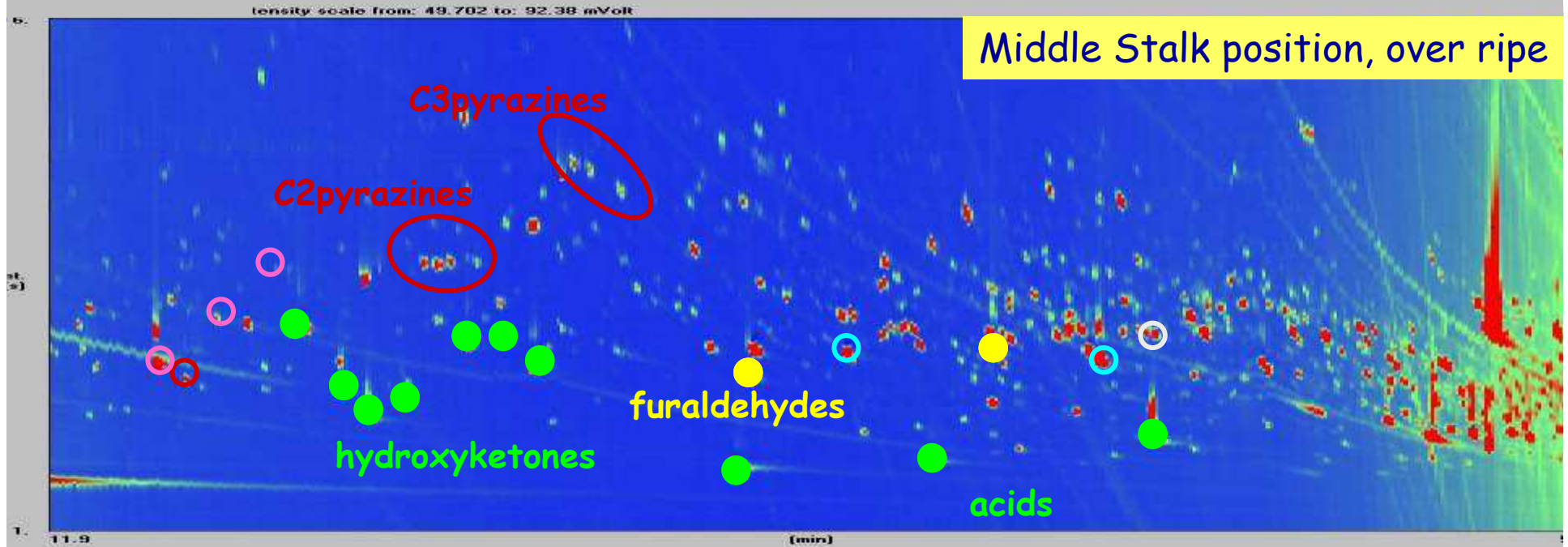
Furfural



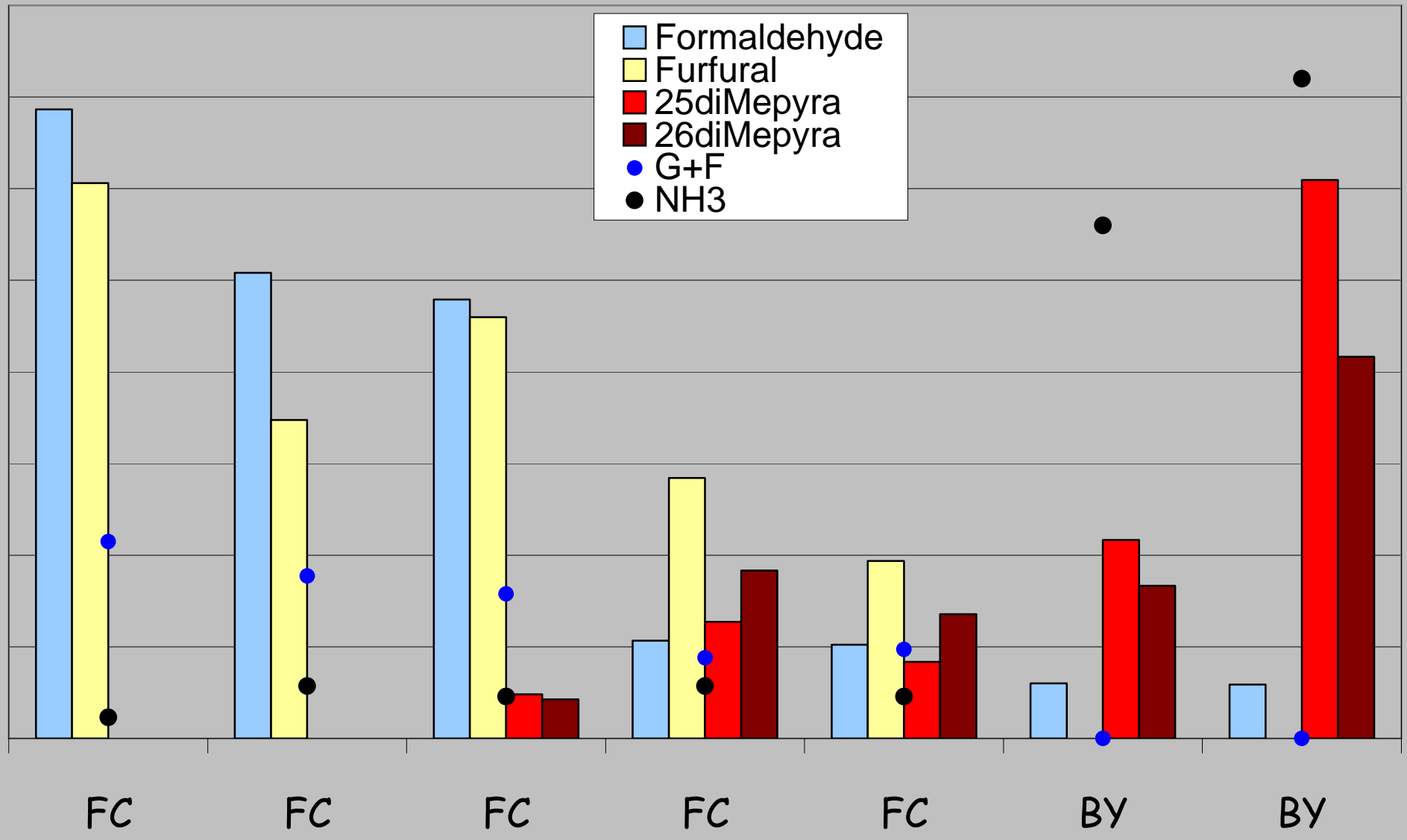
# Tobacco comparison



# Comparison of Flue-Cured

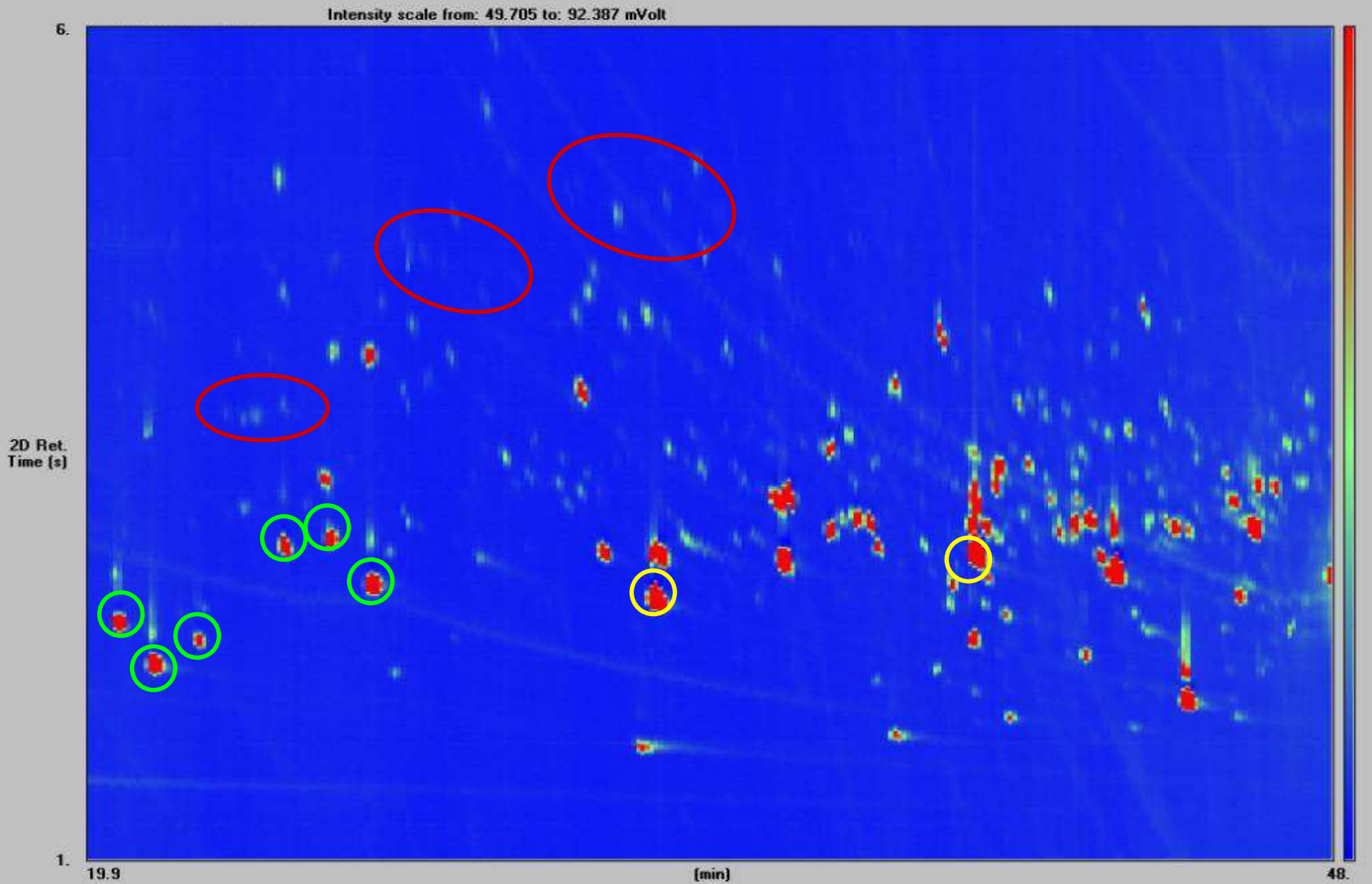


# Link with smoke compounds

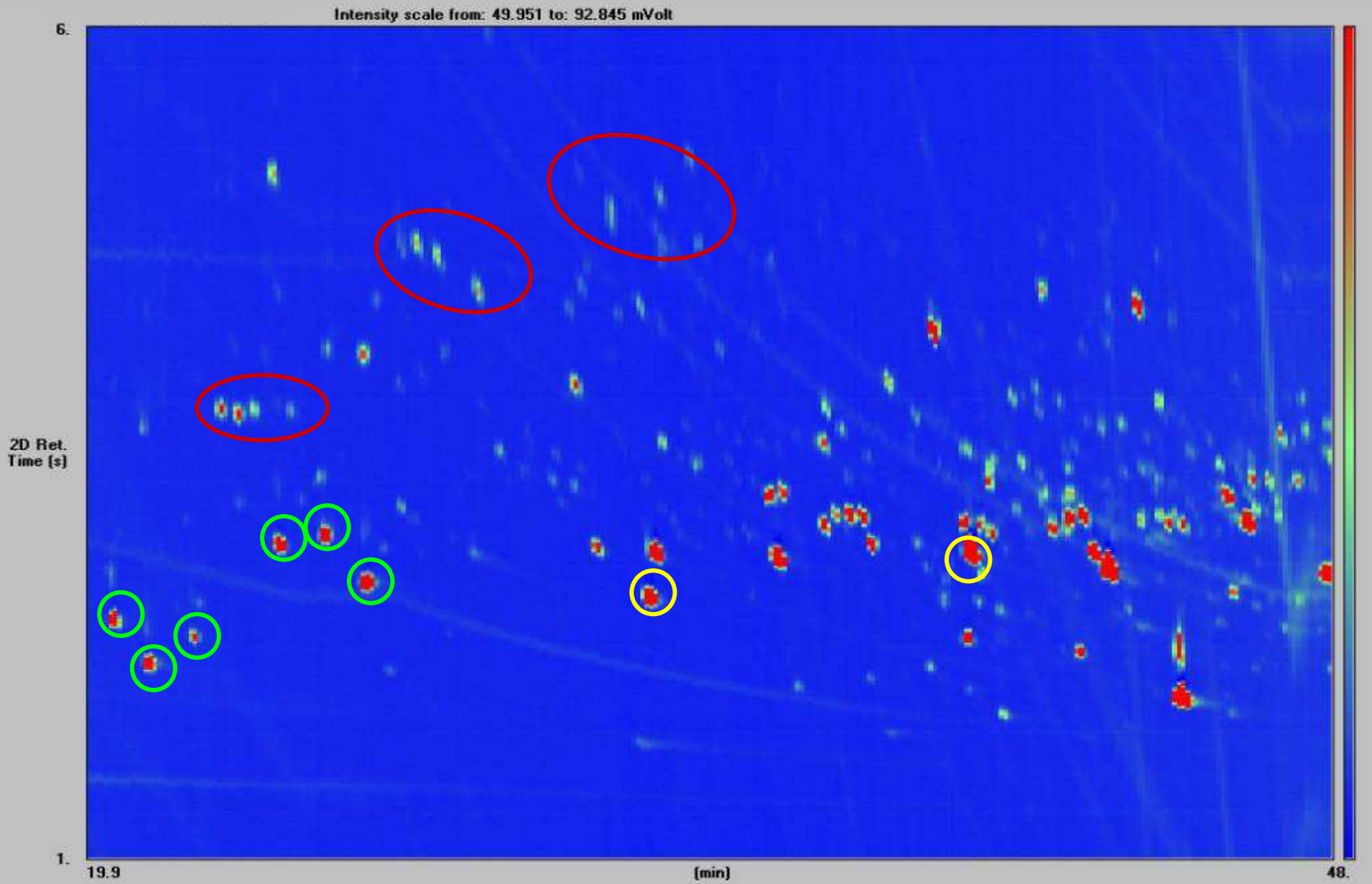




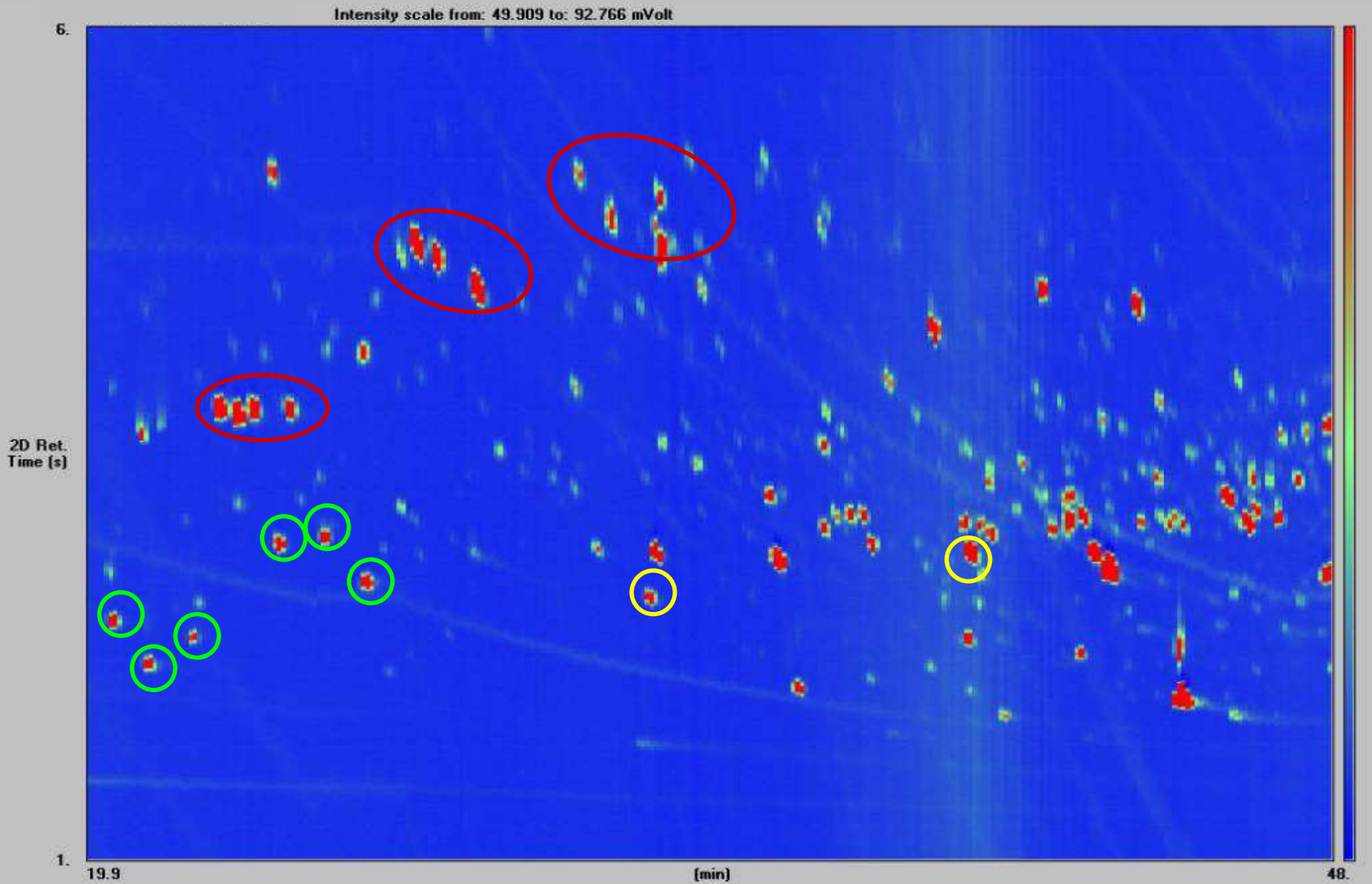
# Interactions between tobaccos : By 0 / FC 100



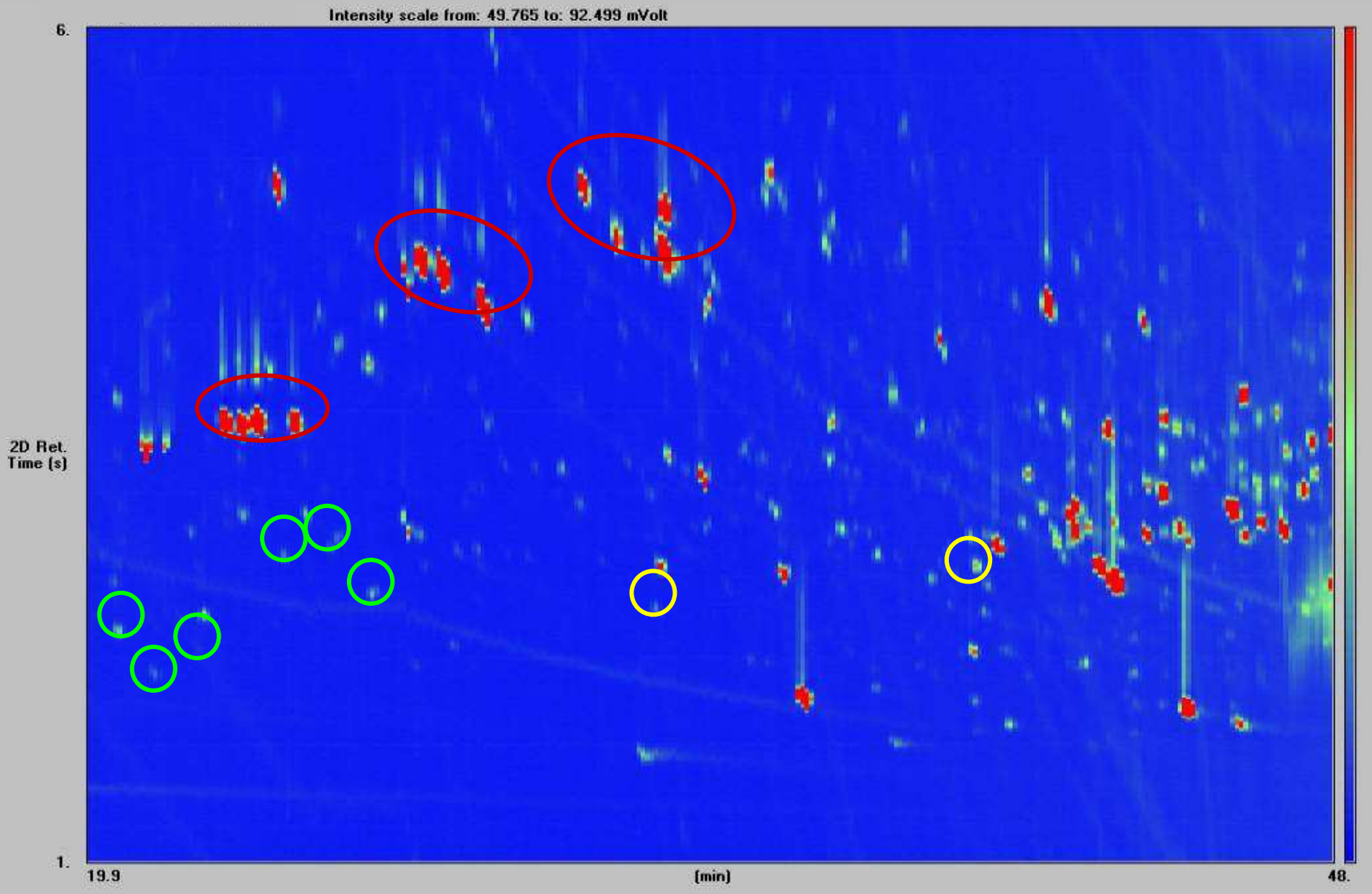
# Interactions between tobaccos : By 25 / FC 75

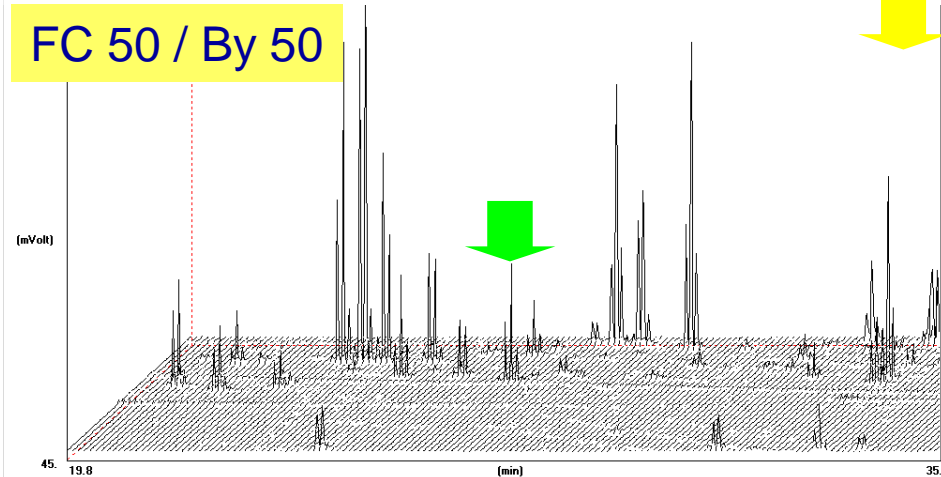
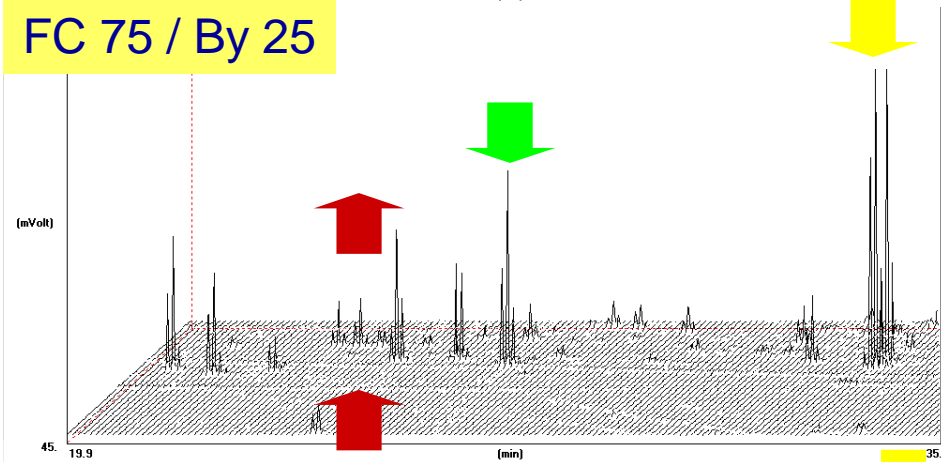
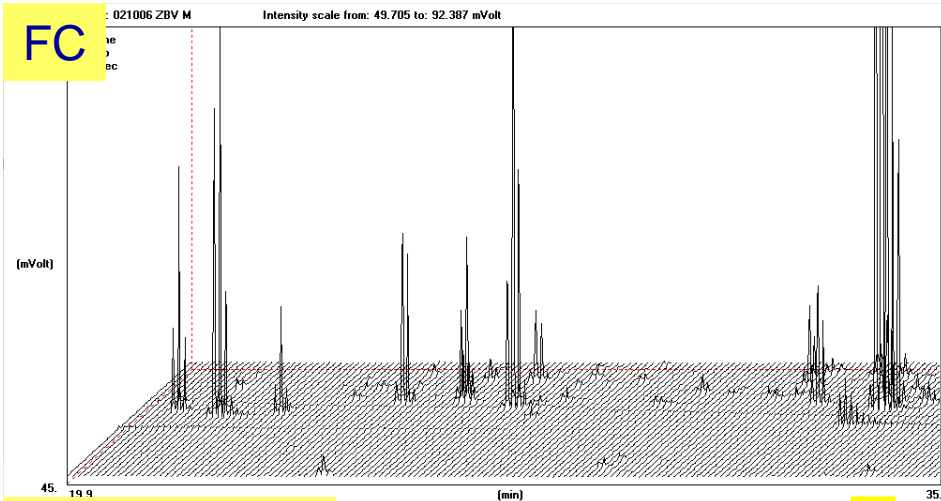


# Interactions between tobaccos : By 50 / FC 50

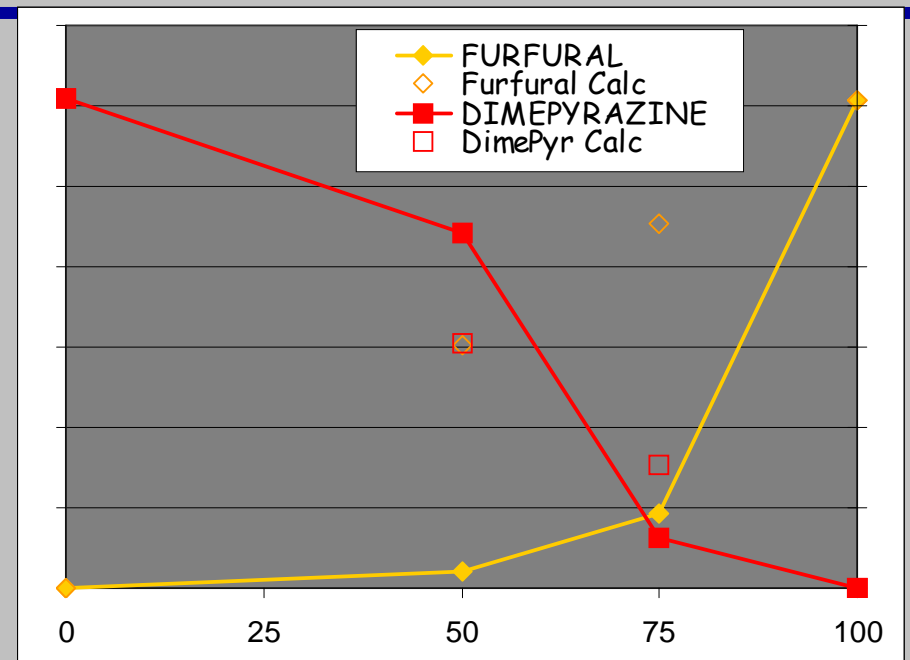


# Interactions between tobaccos : By 100 / FC 0

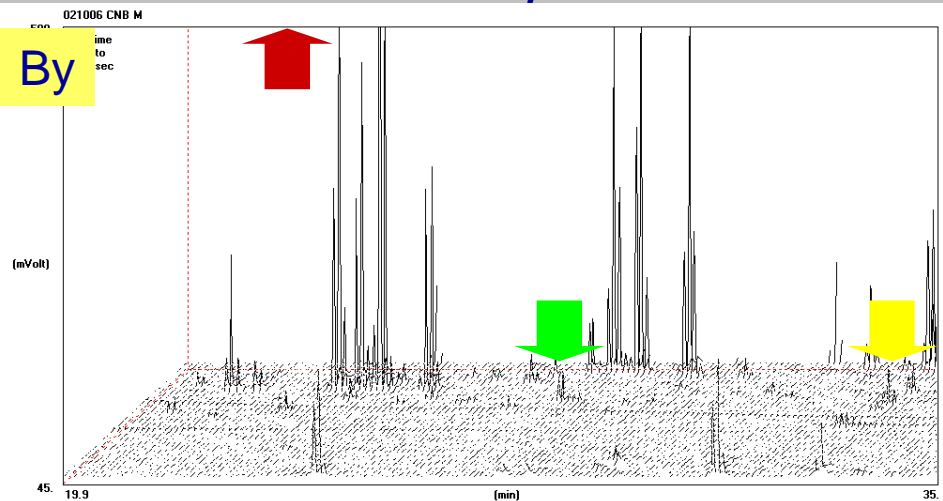




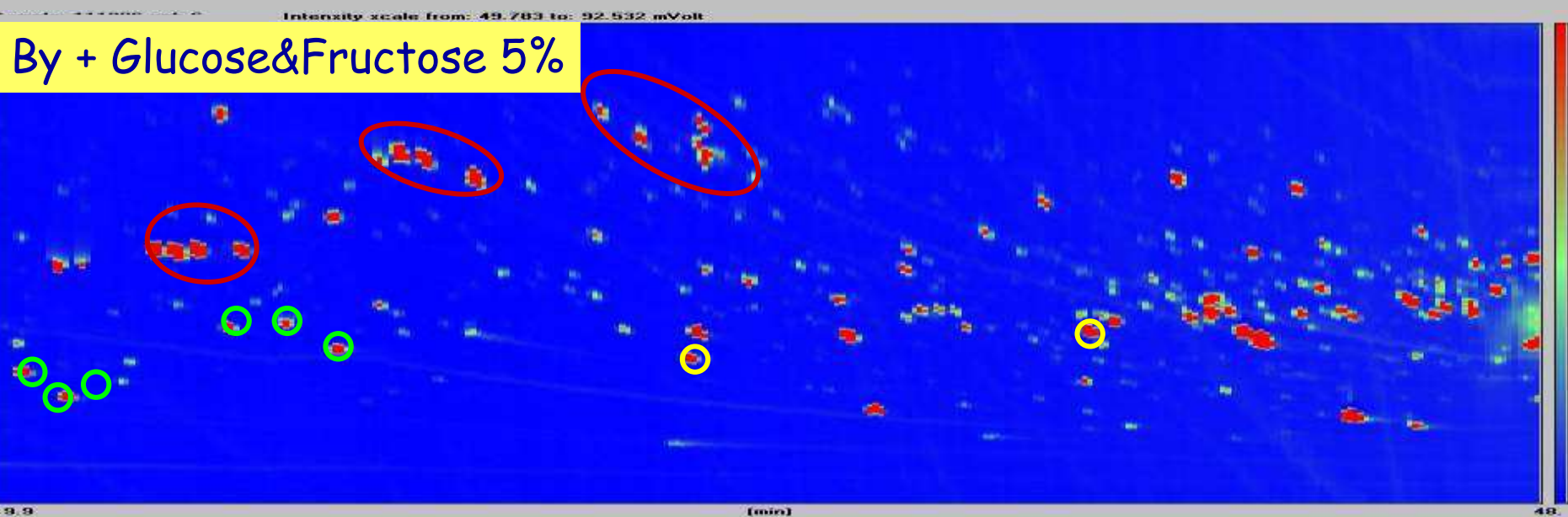
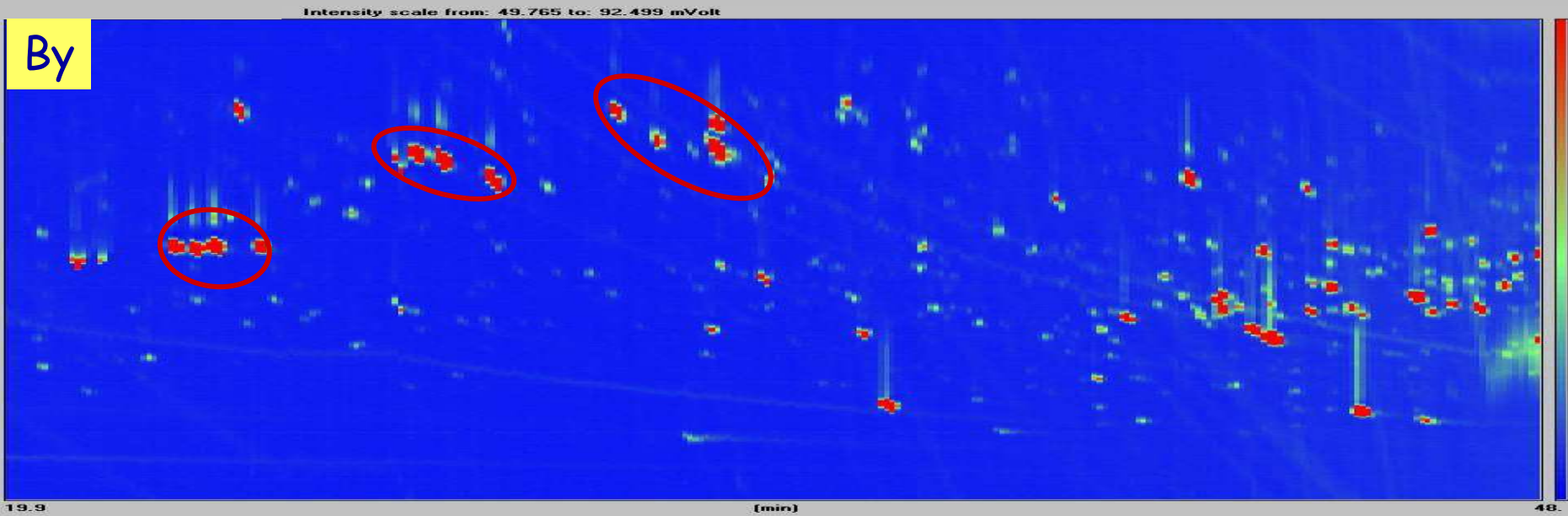
# Interactions By/FC



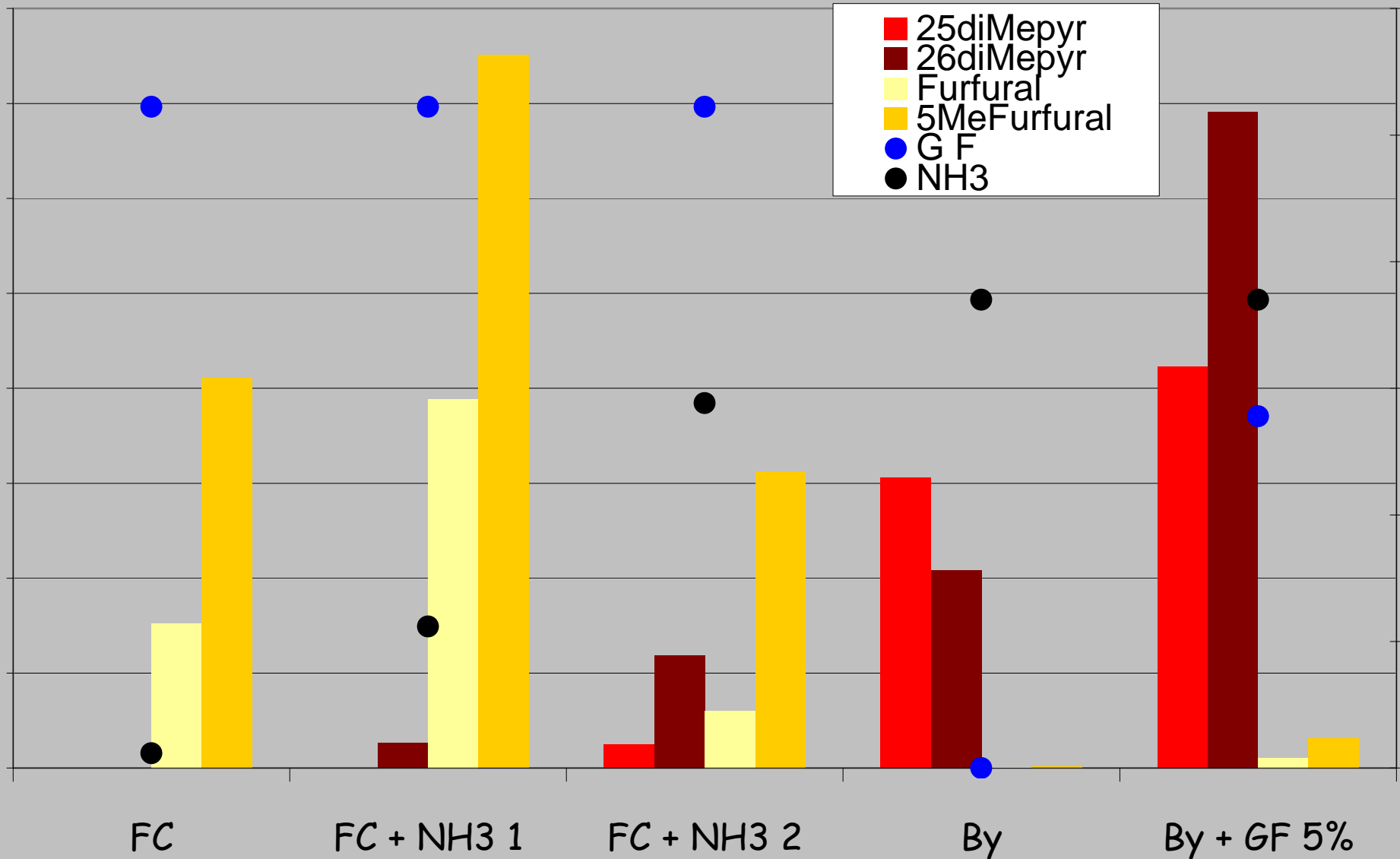
✧ Quick decrease in furfural content with By addition



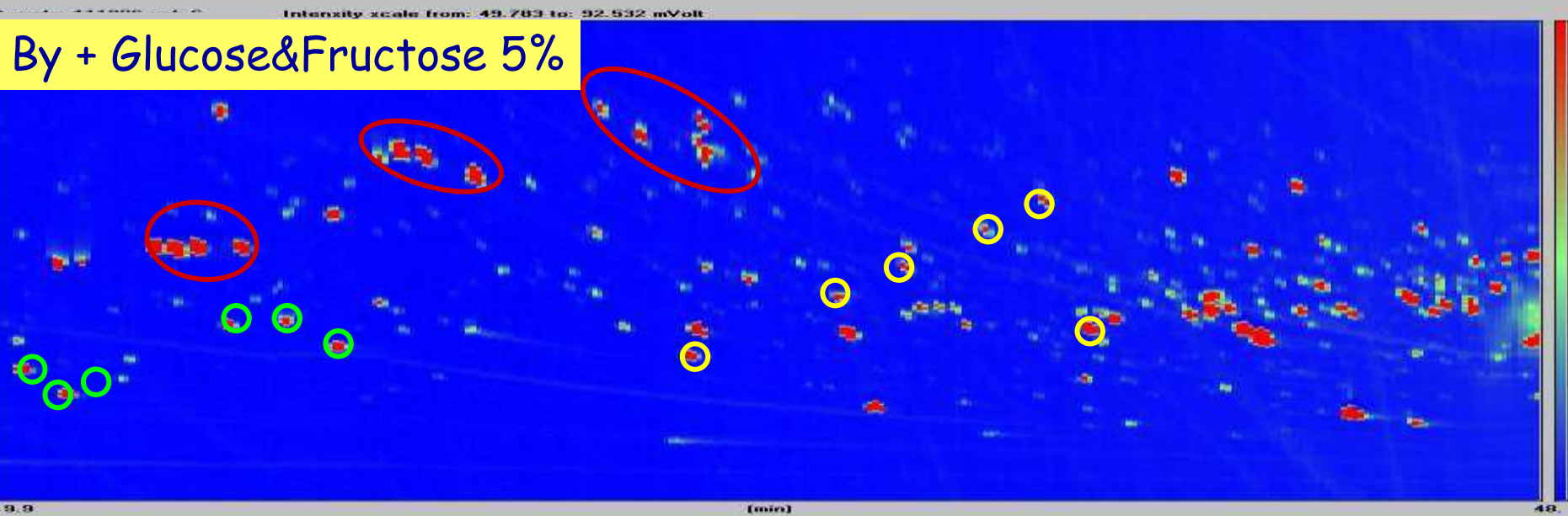
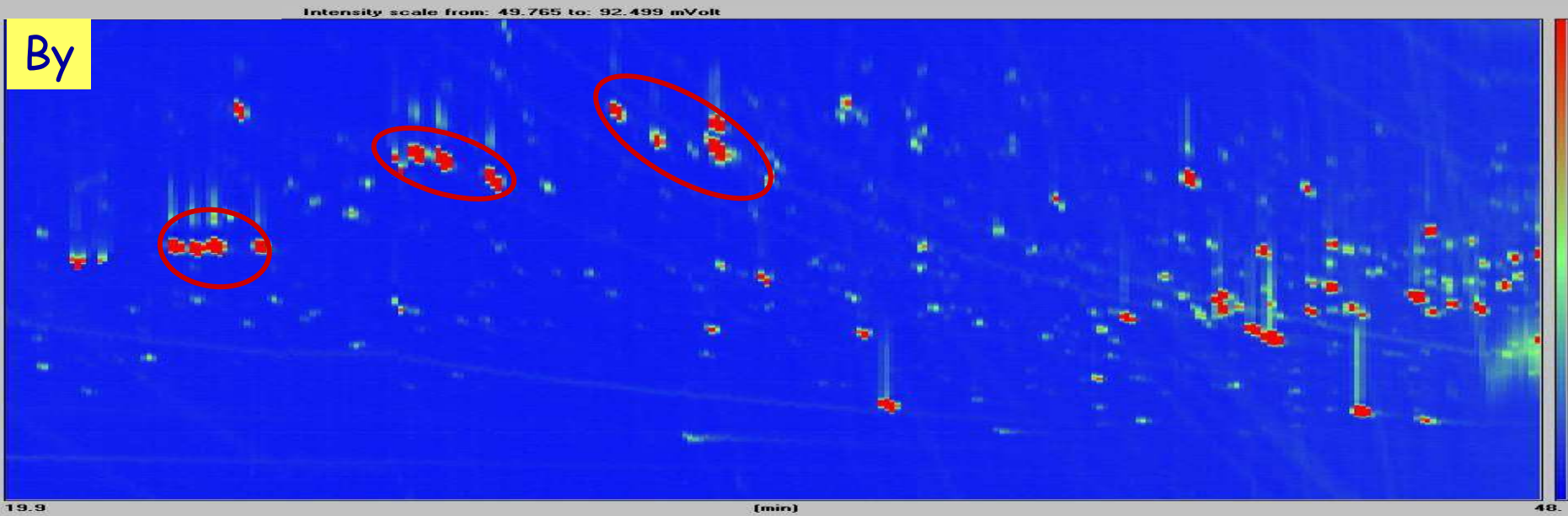
# Additives effect



# Additives effect



# Additives effect





# Conclusion

- ✧ Heating of tobaccos
  - Information on carbohydrate / nitrogenous equilibrium during combustion
  - Link with smoke composition
  
- ✧ GCxGC
  - Improved performance compared to 1D-GC
  - Fingerprint of the prominent families of compounds
  - At a glance visualisation of differences between samples
  - Easier comparison of heated tobacco extracts

Promising tool for the understanding  
of the smoke composition