

# Combustion chemistry of anisole/hydrocarbon fuel mixtures under flame conditions

Presented by: Kanika Sood,  
Collaborators: Sylvie Gosselin, Abderrahman El Bakali,  
Supervisors: Laurent Gasnot, Luc-Sy Tran

**Réunion du comité français de la FRIF  
12 Mai, 2022**



# Plan of the presentation

- Context/Objective
- Methodology/Experimental setup
- Flame conditions
- Flame measurements
- Selected Results
- Perspectives

# Context



Global Warming

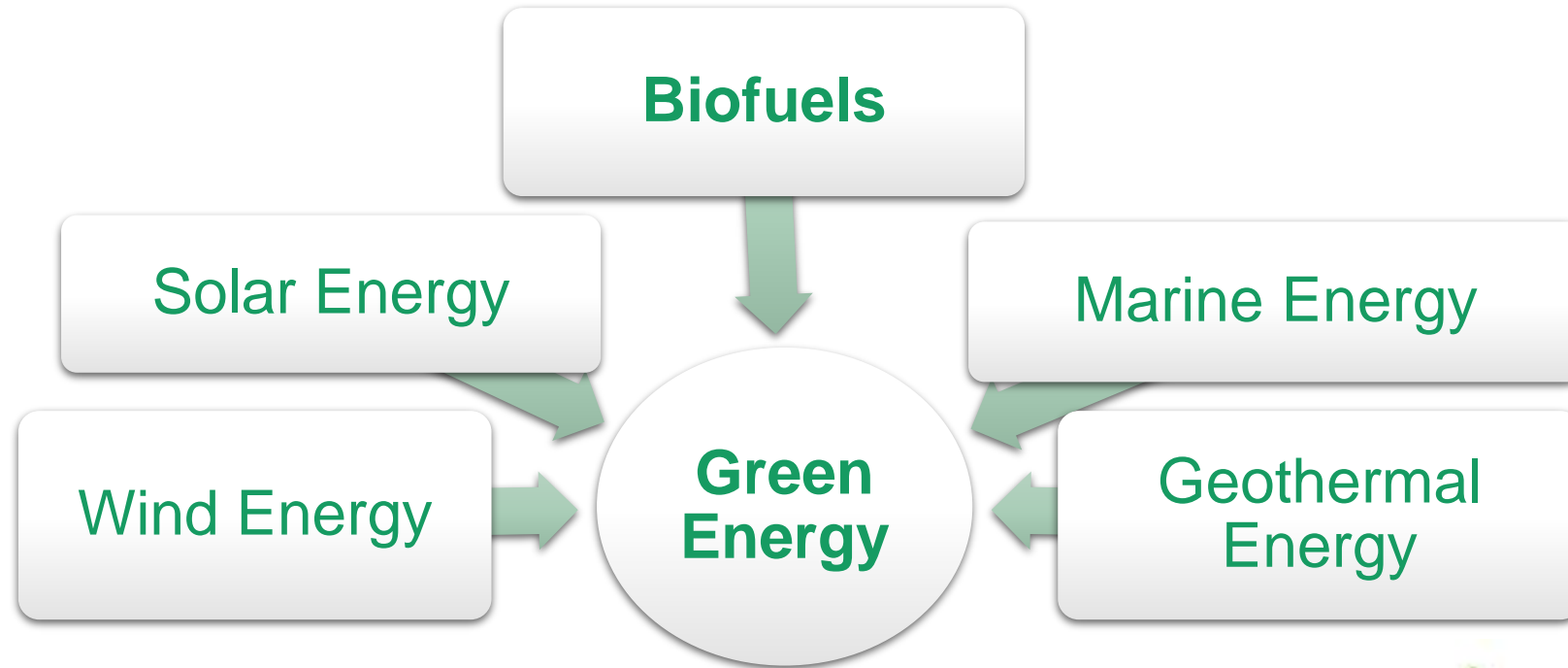


Respiratory diseases



- Global energy production from the combustion of fossil fuels ~ **80% !!!!**

# Context

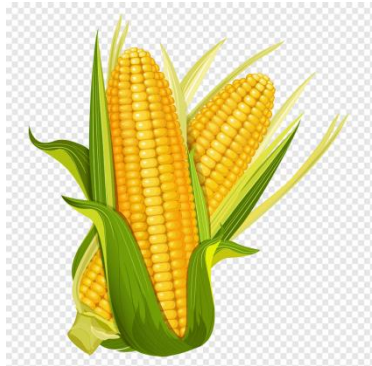


Due to:

- Increase in energy demand
  - Ecological demand to reduce emissions
  - Economic demand to increase efficiency
- « It is necessary to investigate **biofuels** ».



# Types of biofuels



## 1st GENERATION

- **Edible biomass**
- Crops/Sugar cane



## 2<sup>nd</sup> GENERATION

- **Non-edible biomass**
- Wood/Straw



## 3<sup>rd</sup> GENERATION

- **Marine**
- Algae/Seaweed

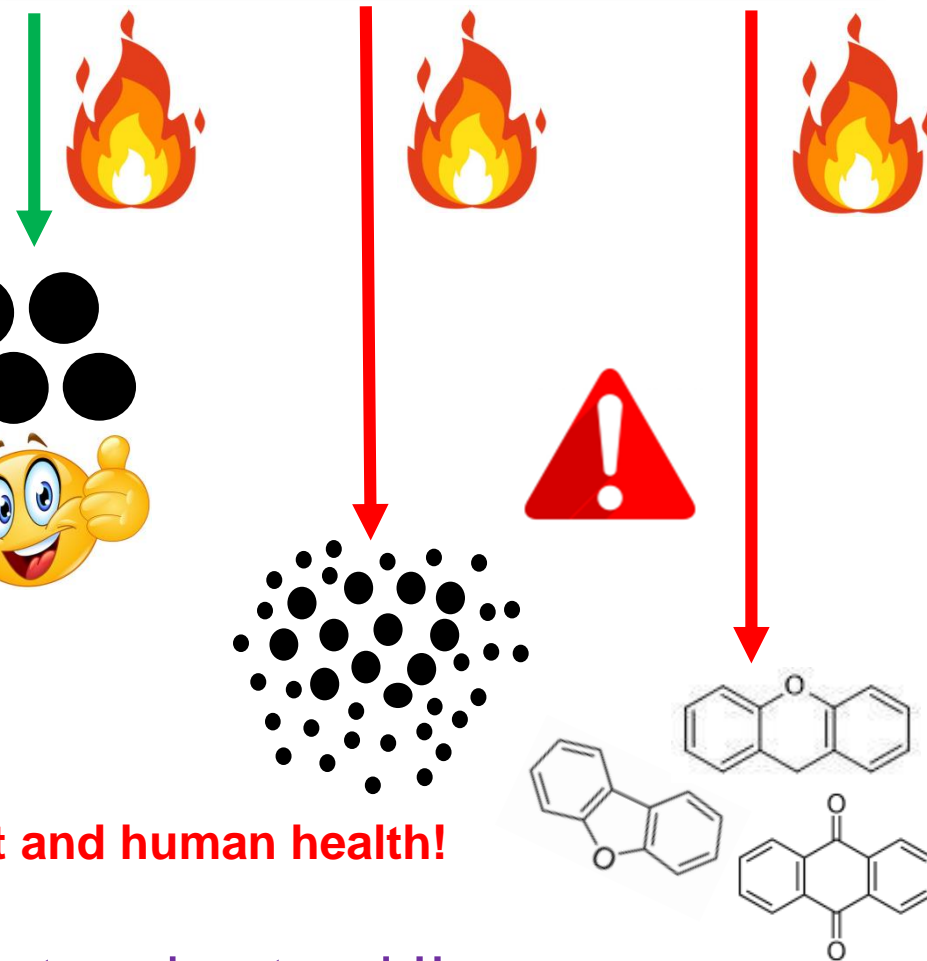
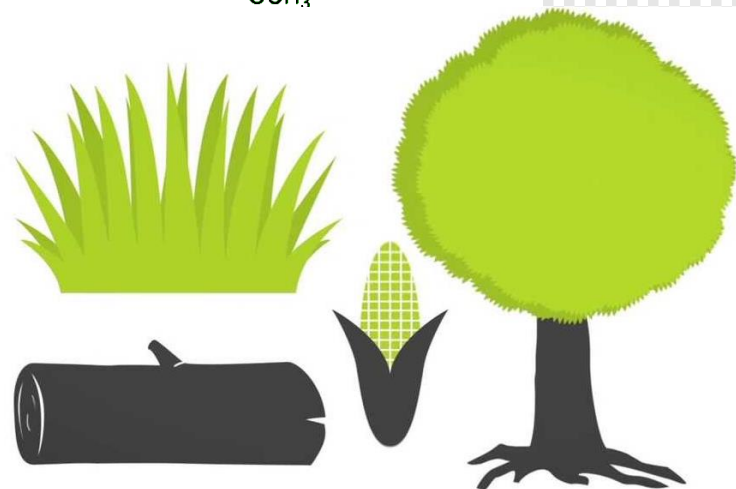
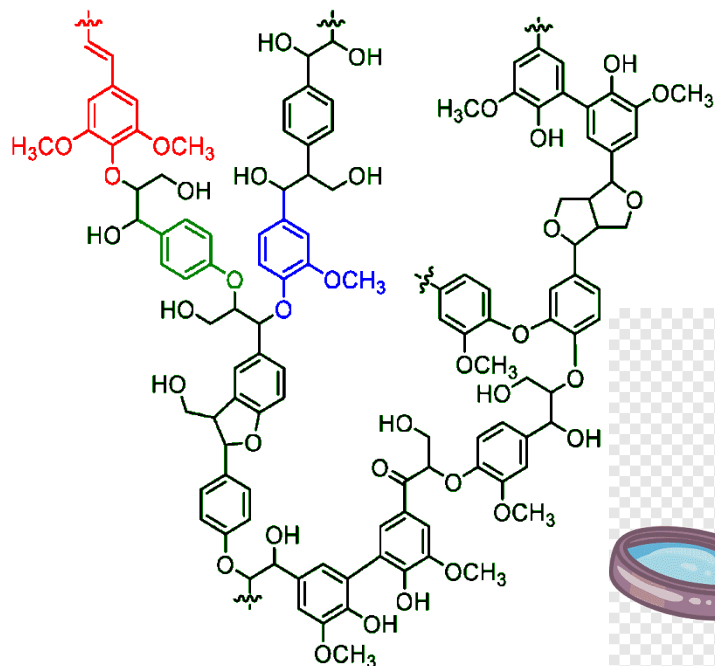
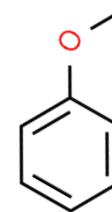


## 4<sup>th</sup> GENERATION

- **Breakthrough**
- Advanced algae

# Context and Objective

Oxygenated **biofuels**  
(contain one or more O atoms)



**Impact on the environment and human health!**

**Fundamentals still not understood !!**

- Zhang et al. *Environ. Sci. Technol.* 2014, 48, 14805-14813
- Sirignano et al. *Exp. Therm. Fluid. Sci. Technol.* 2018, 95, 60-64

- Guan et al. *Atmospheric Pollution Research* 2017, 8, 209-220

**As part of this project, we plan to answer the following questions:**

How do oxygenated biofuels participate in the production of **OPAHs**?



What are the chemical **structures** of OPAHs? How **OPAHs react** and participate in the formation of **small soot particles**?

# Approach and Methodology

- Biofuels to be studied:**

Mixture 1 - Isooctane/Anisole

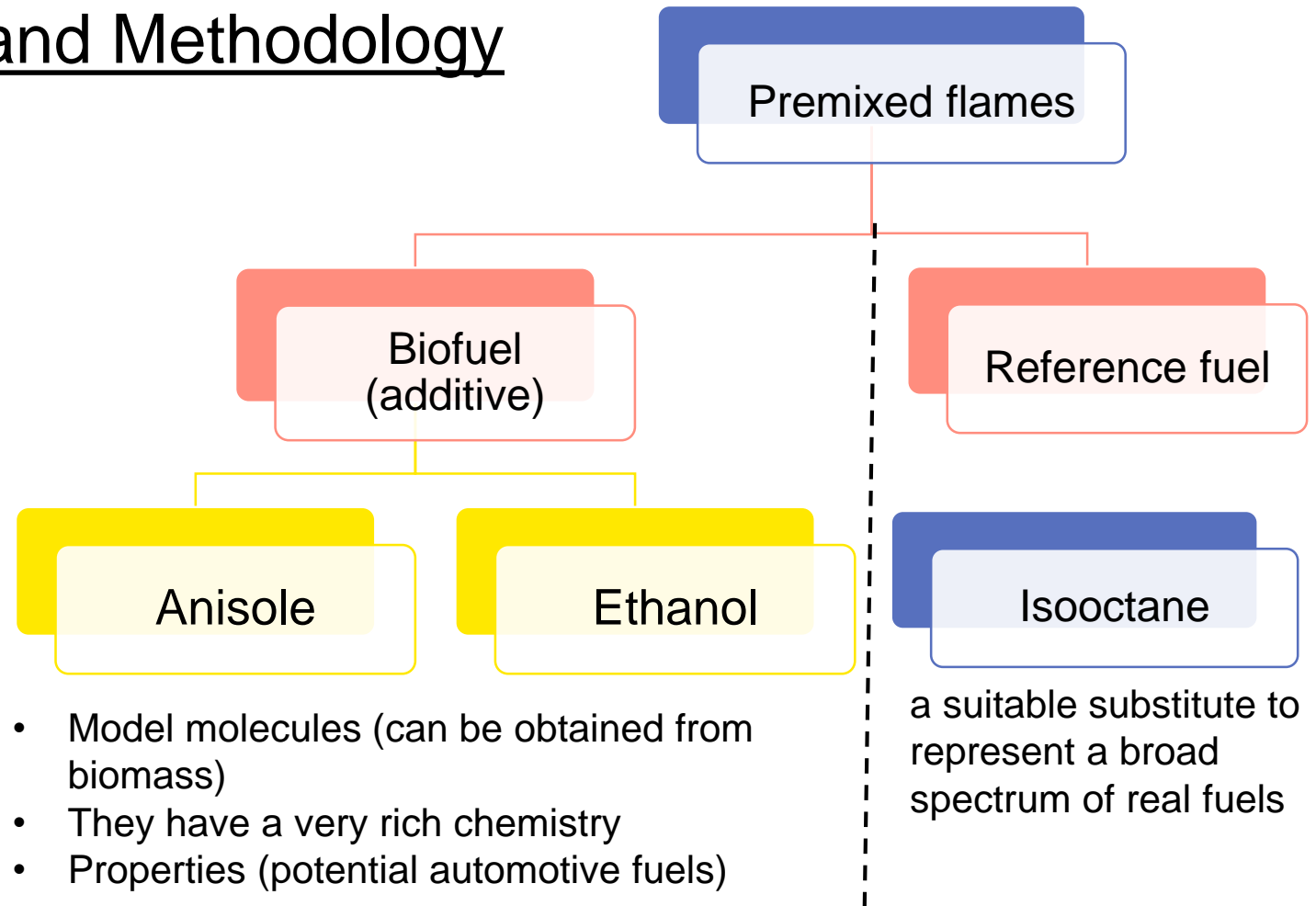
Mixture 2 - Isooctane/Ethanol

Mixture 3 - Isooctane/2,5-dimethyl Furan

- Approches to be used:**

Experiments (Premixed flames)

Simulations (Kinetic Modeling)

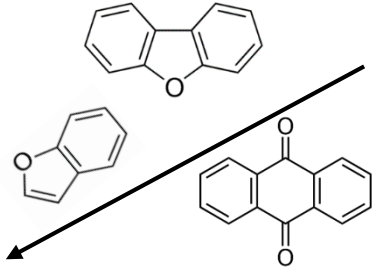


Fuel	Lower Heating Value (MJ/L)	Octane Number
Gasoline	42	95
Ethanol	27	109
Anisole	33	103

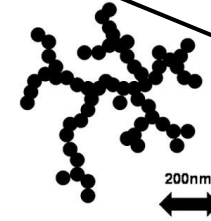


## GC-SCION

- ❑ Advanced SPT technology ~ 1 ppb!
- ❑ TCD/FID detectors



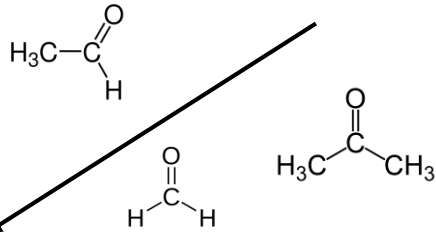
- ❑ Scanning mobility Particle Sizer
- ❑ Can measure until 1 nm



## SMPS-1nm

## GC-Perkin

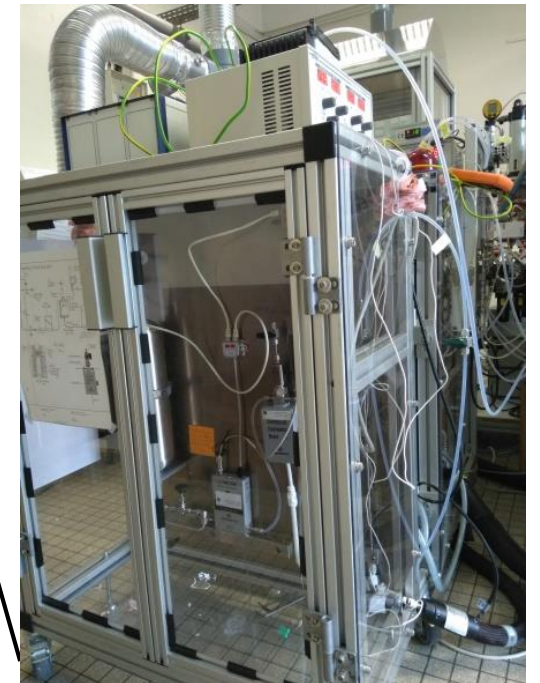
- ❑ FID with **Methanizer**
- ❑ Detects aldehydes (HCHO), ketone, etc.!



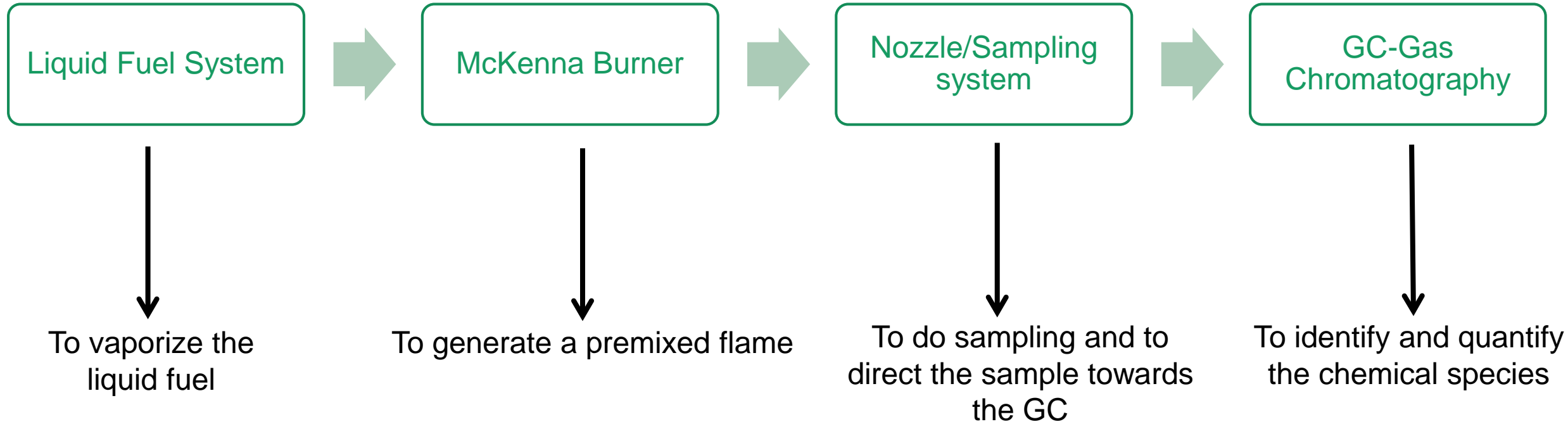
## GC-MS Agilent

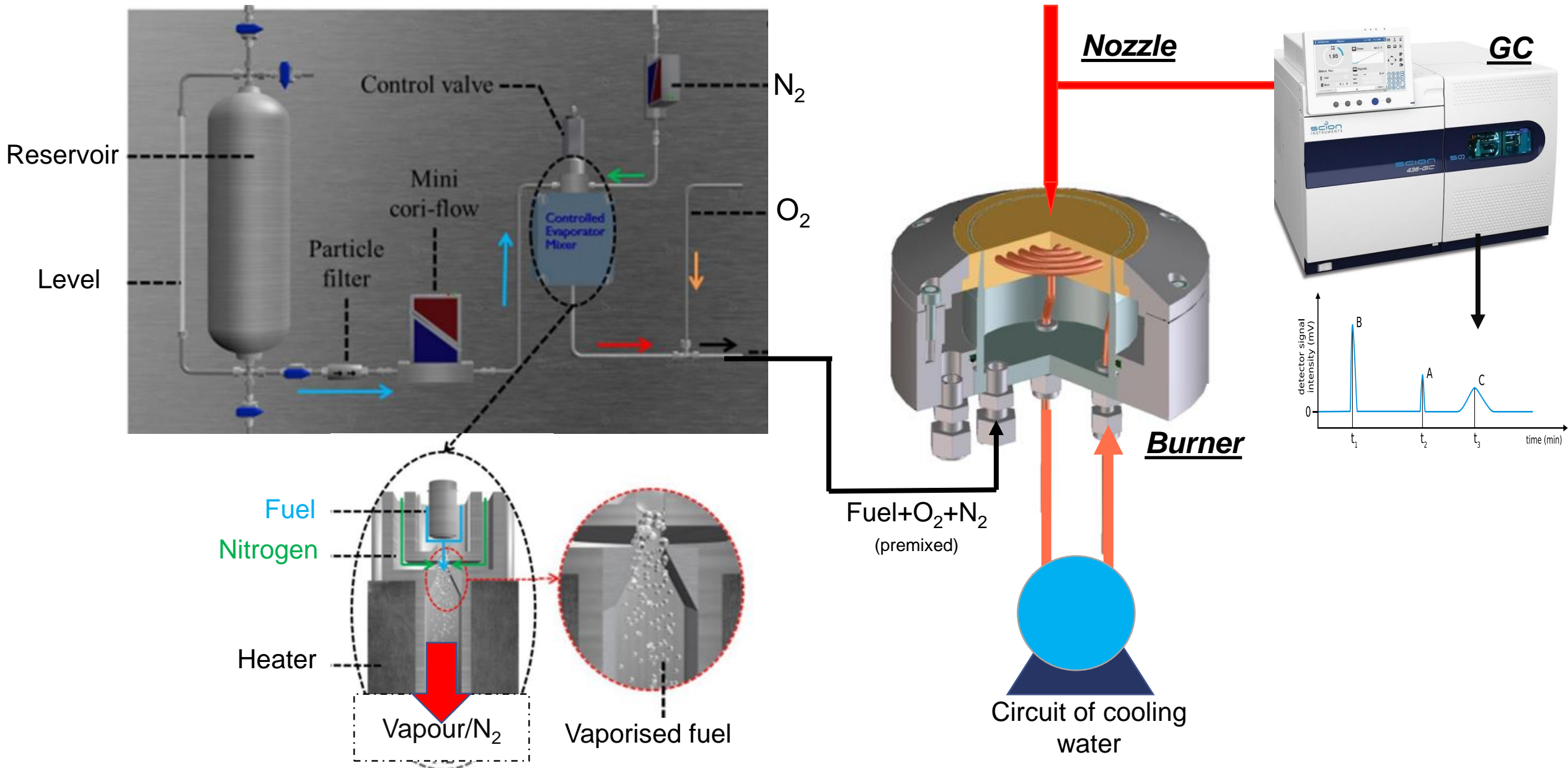


# Experimental Room



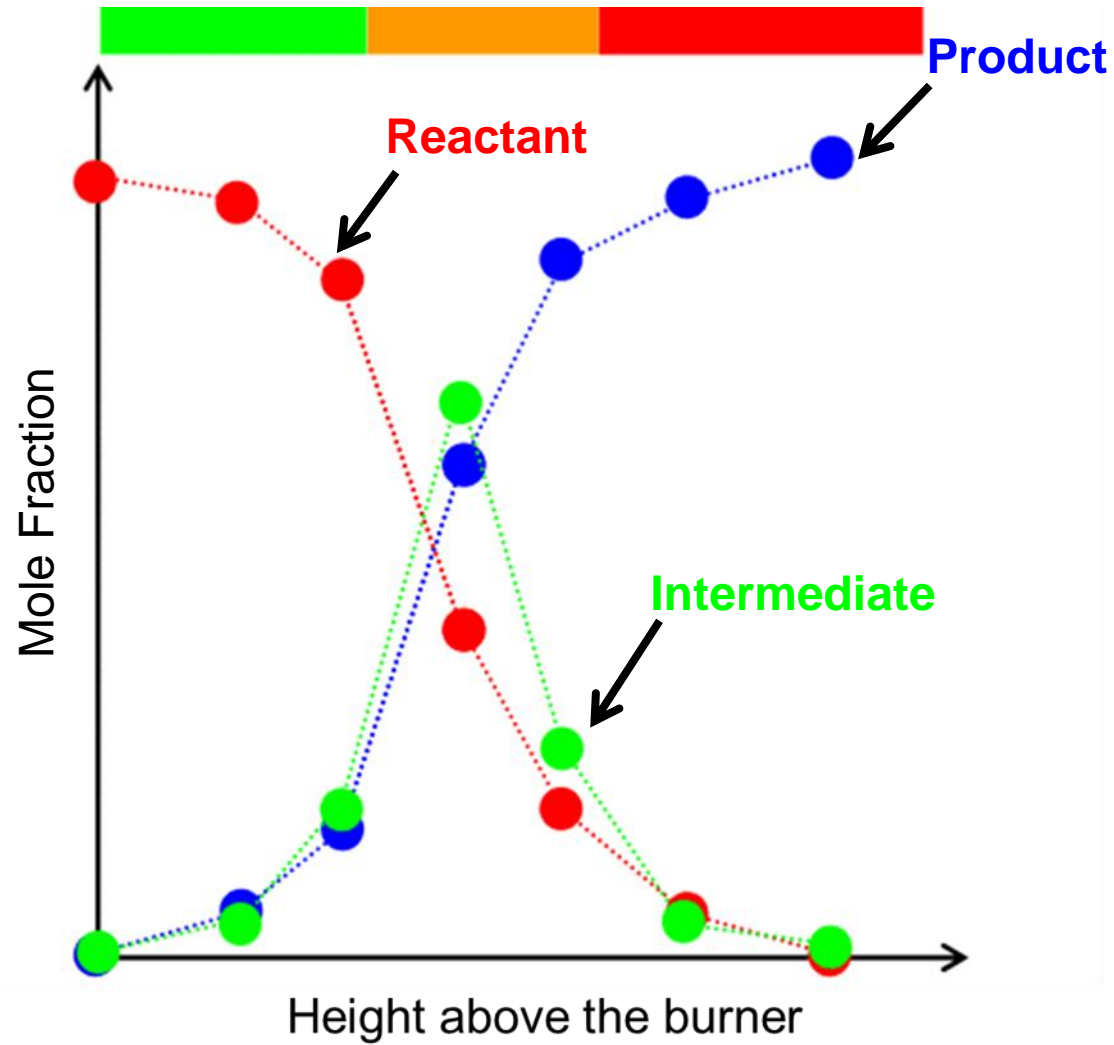
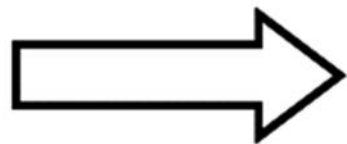
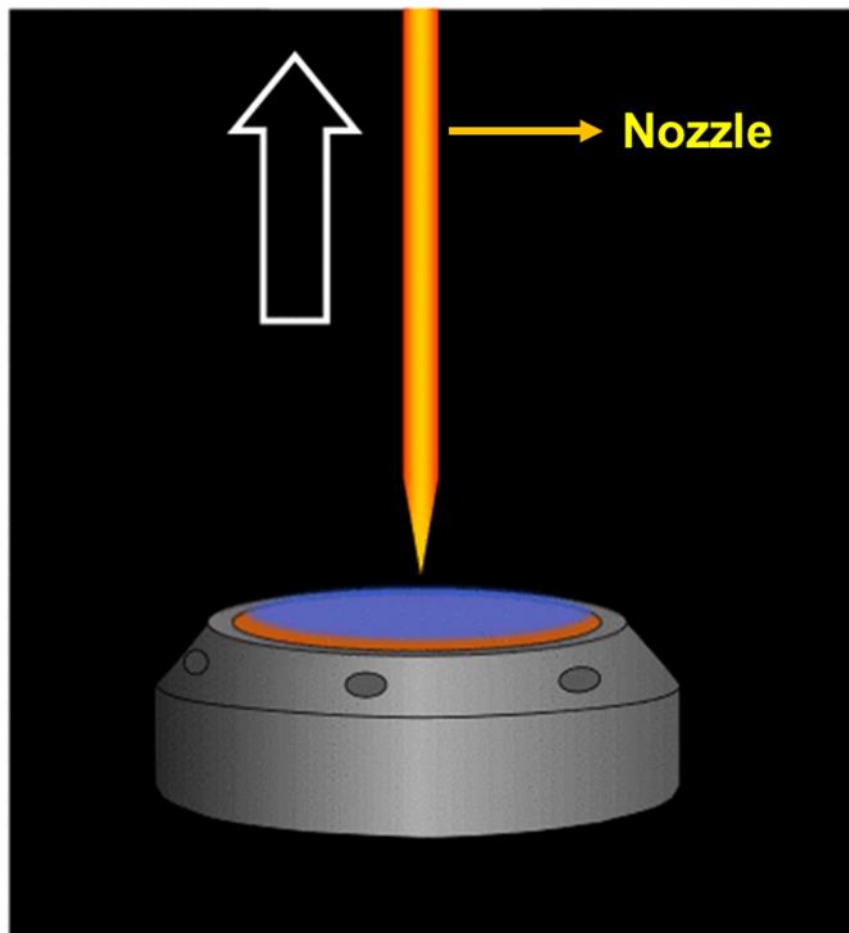
# Global Scheme of the Flame-GC System



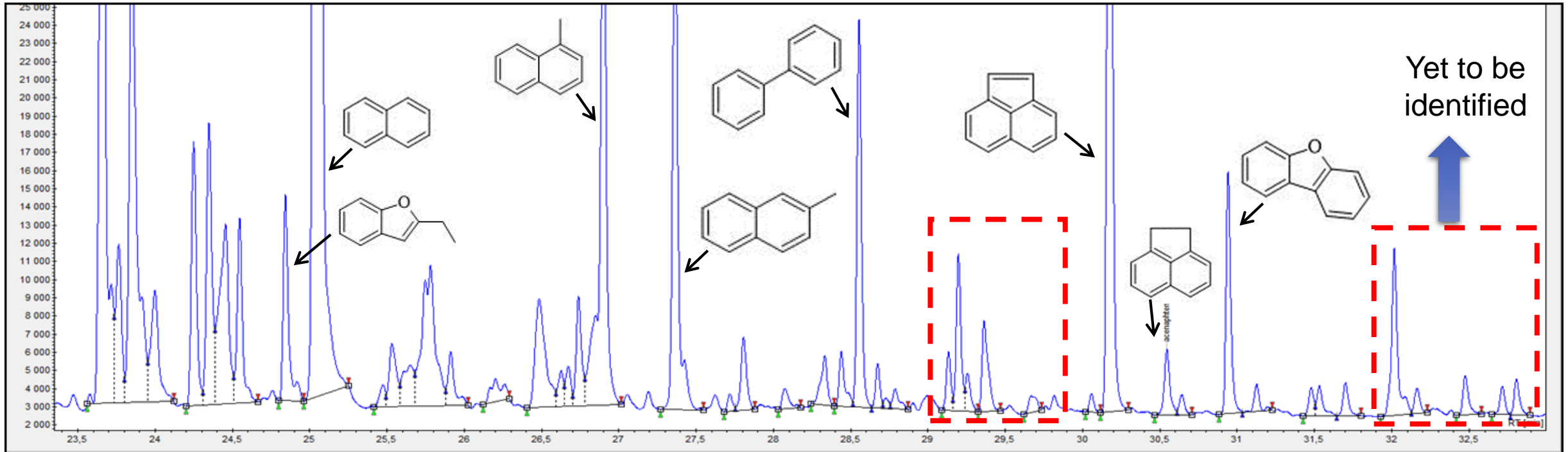


**Liquid Fuel System**

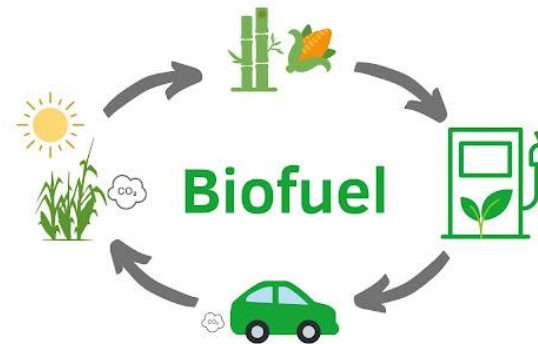
# Sampling System



# An example of a chromatogram ...

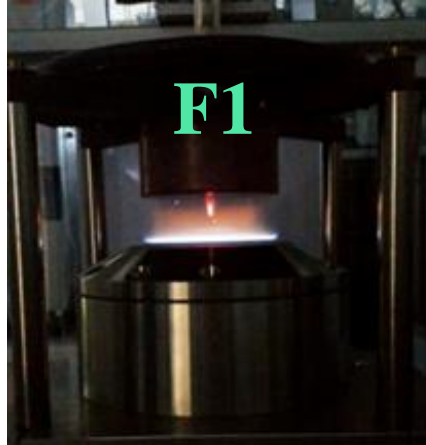


Anisole flame  
(PC2A)



# Flame Conditions

## Series 1



Equivalence Ratio = **1.82**  
Anisole = **0%**



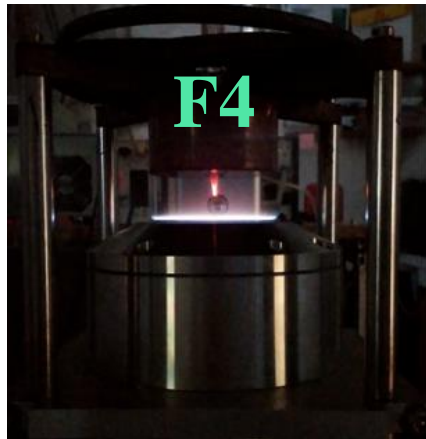
Equivalence Ratio = **1.82**  
Anisole = **10%**



Equivalence Ratio = **1.82**  
Anisole = **15%**

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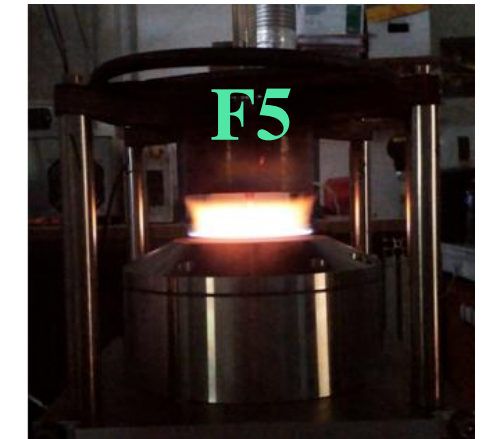
## Series 2



Equivalence Ratio = **1.7**  
Anisole = **10%**



Equivalence Ratio = **1.82**  
Anisole = **10%**



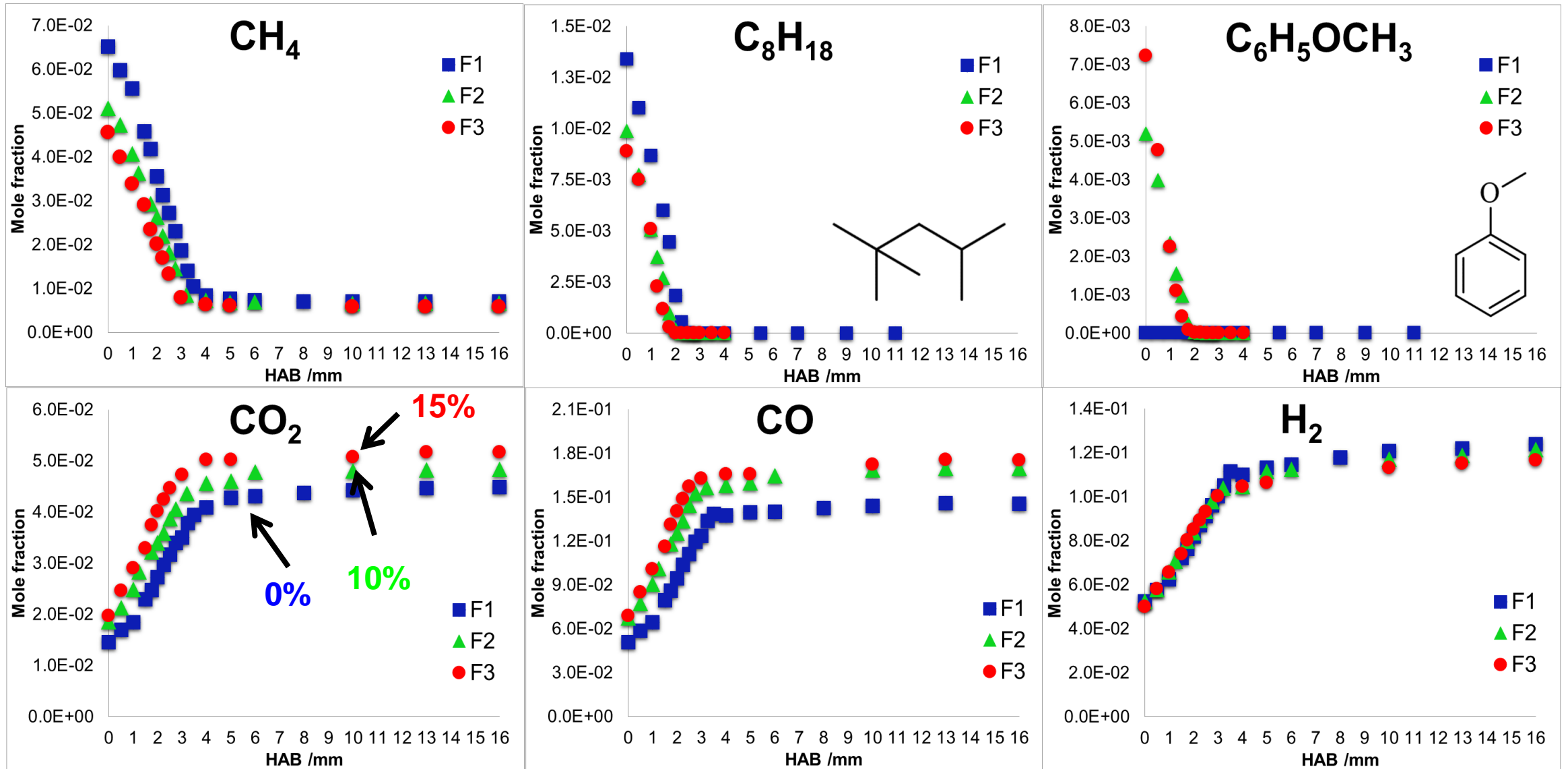
Equivalence Ratio = **1.9**  
Anisole = **10%**

# Preliminary Results

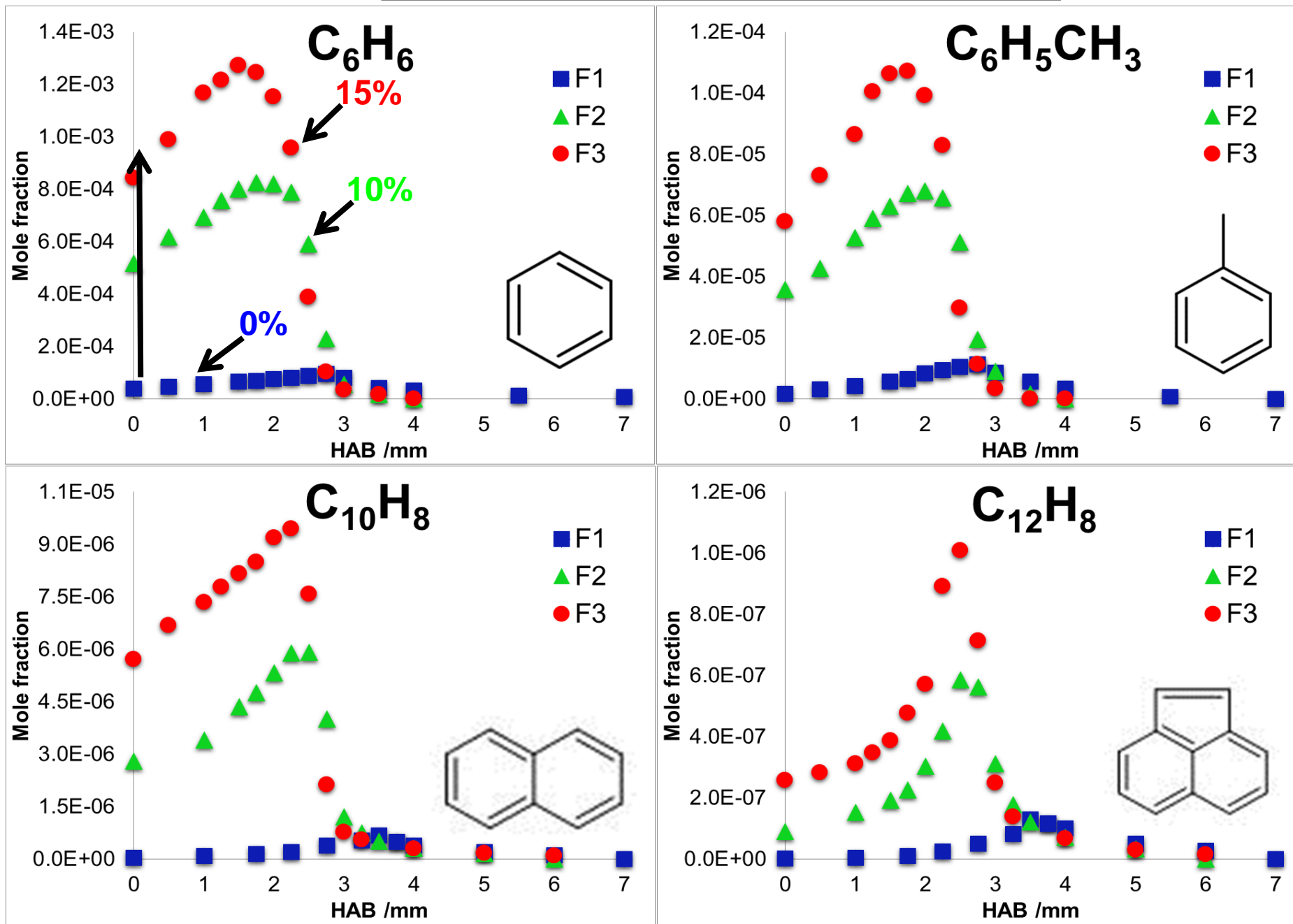




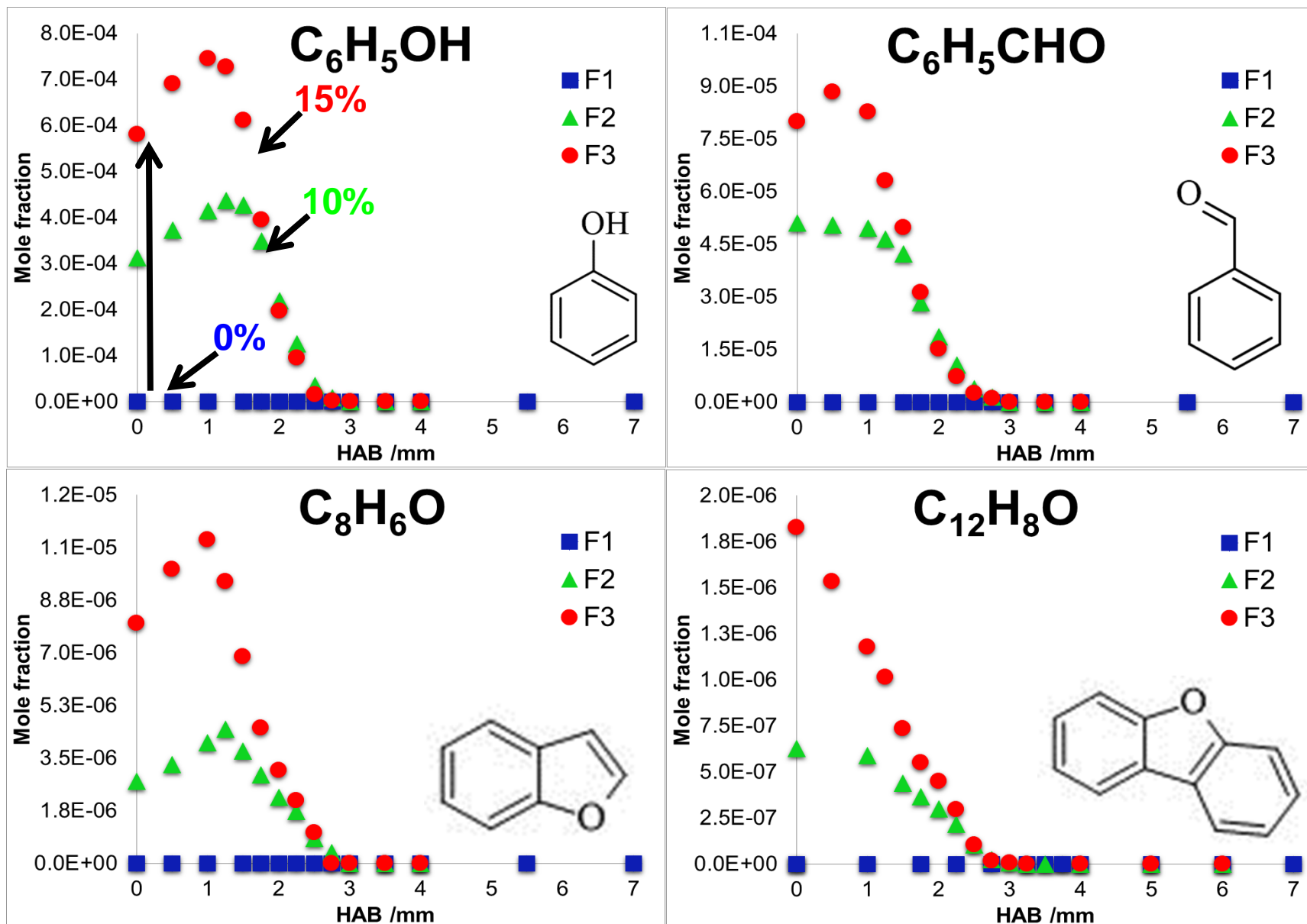
# Selected Results: Series 1



# Selected aromatics: Series 1

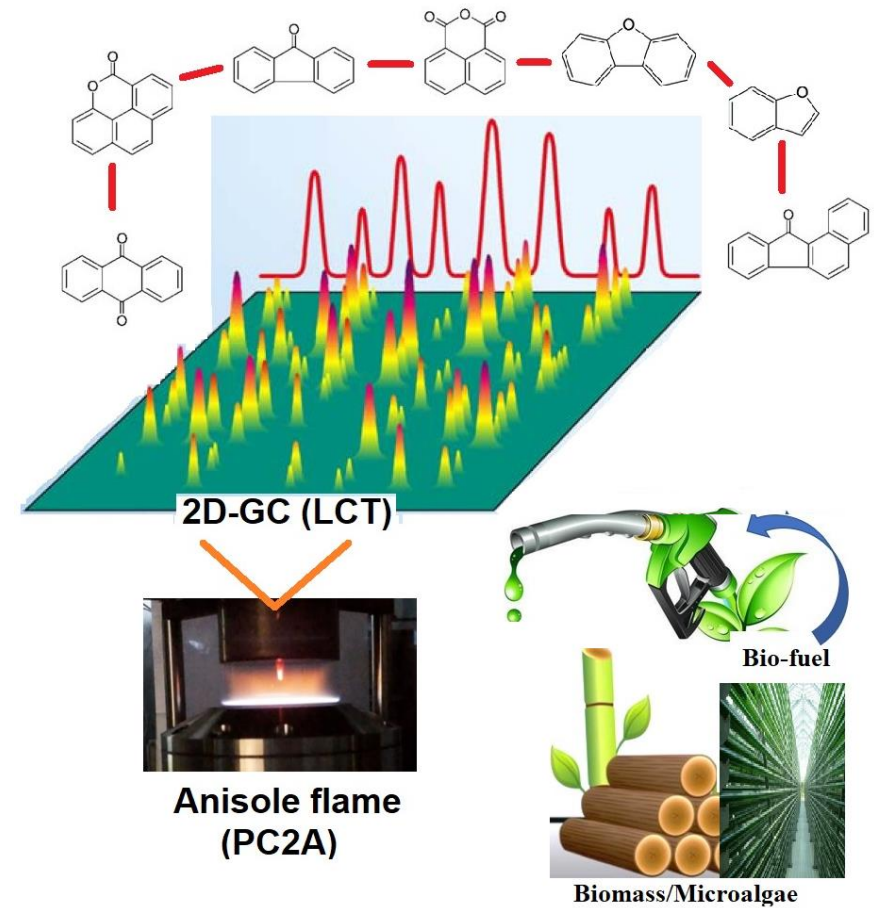


# Selected oxy-aromatics: Series 1



## Next Steps ...

- 2D-GC measurements (in June; Ghent, Belgium)
- Comparison with other biofuels (ethanol, DMF)
- SMPS for soot particle size measurements (coll. P. Desgroux and A. Faccinetto)
- Temperature measurements (coll. P. Desgroux and X. Mercier)
- Modeling of combustion of biofuels (coll. J.C. Lizardo-Huerta)



**Merci pour votre attention**