Combustion chemistry of anisole/hydrocarbon fuel mixtures under flame conditions

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Plan of the presentation

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

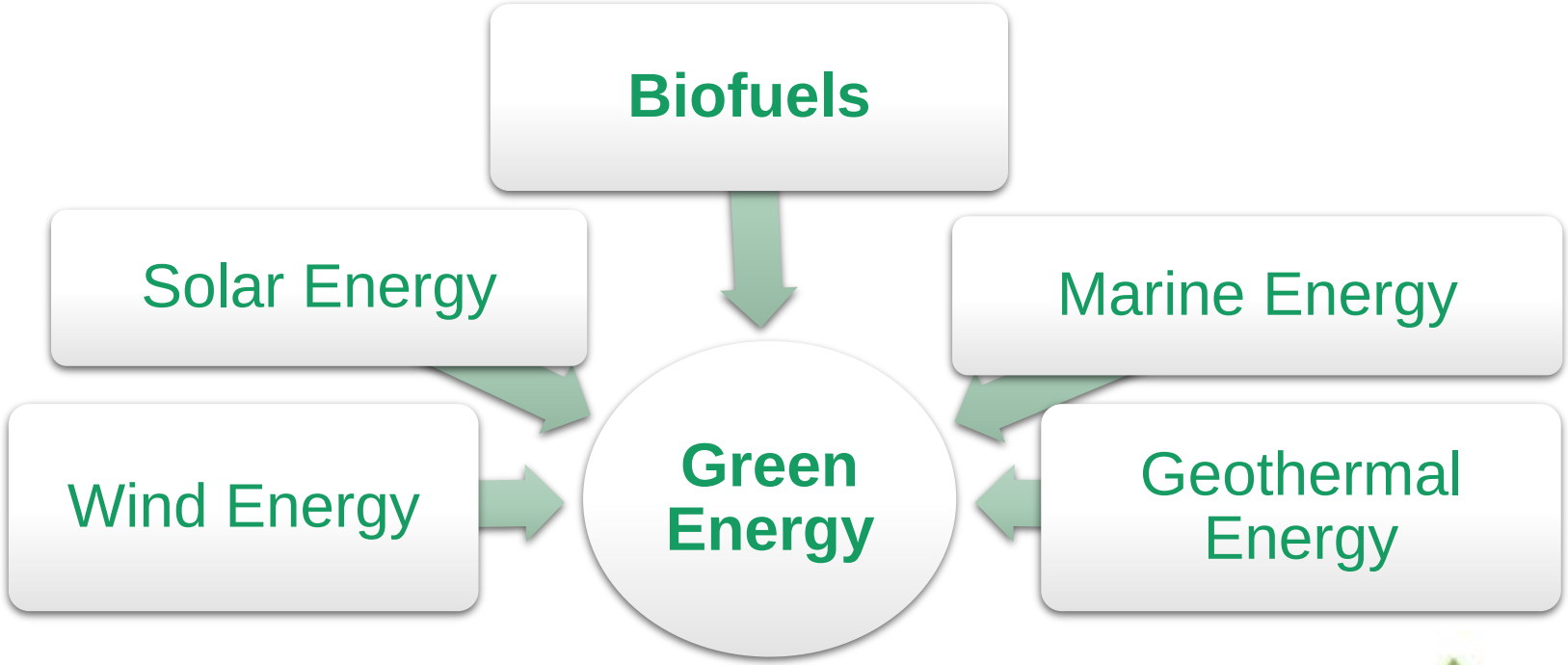
Context

Global Warming

Respiratory diseases

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

Context

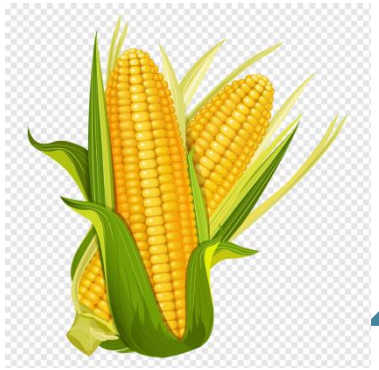


Due to:

- Increase in energy demand
- Ecological demand to reduce emissions
- Economic demand to increase efficiency

« It is necessary to investigate **biofuels** ».

Types of biofuels



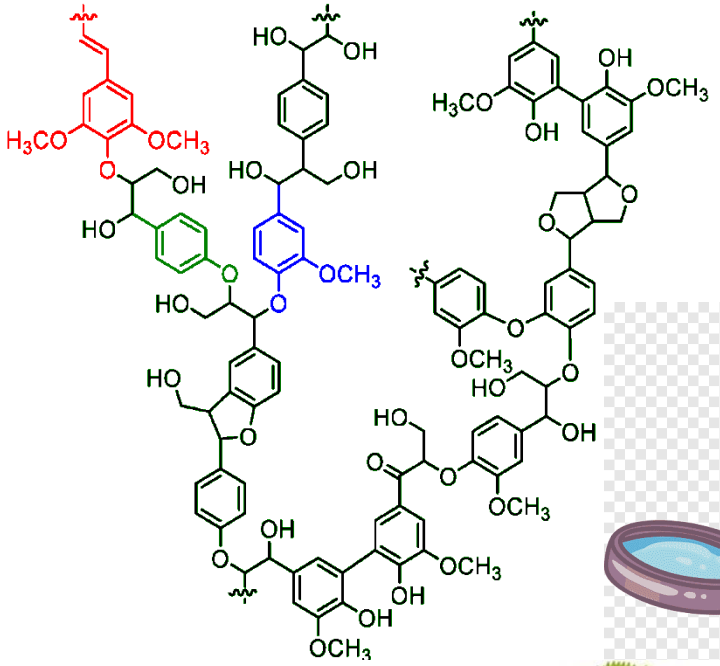
1st GENERATION
- **Edible biomass**
- Crops/Sugar cane

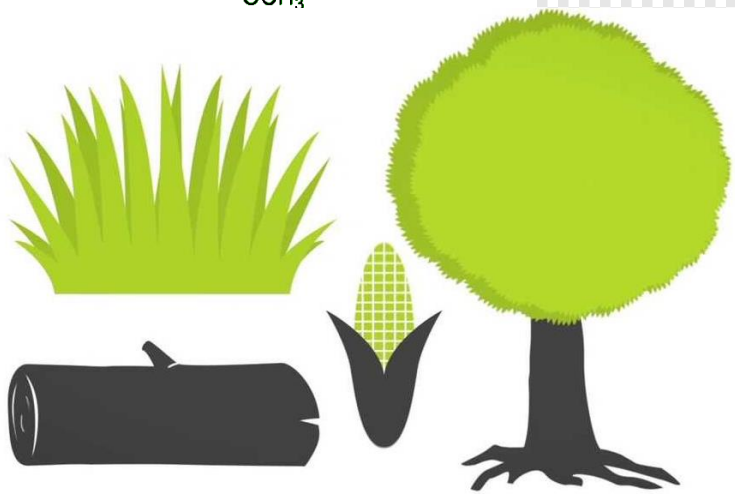
2nd GENERATION
- **Non-edible biomass**
- Wood/Straw

3rd GENERATION
- **Marine**
- Algae/Seaweed

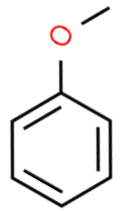
4th GENERATION
- **Breakthrough**
- Advanced algae

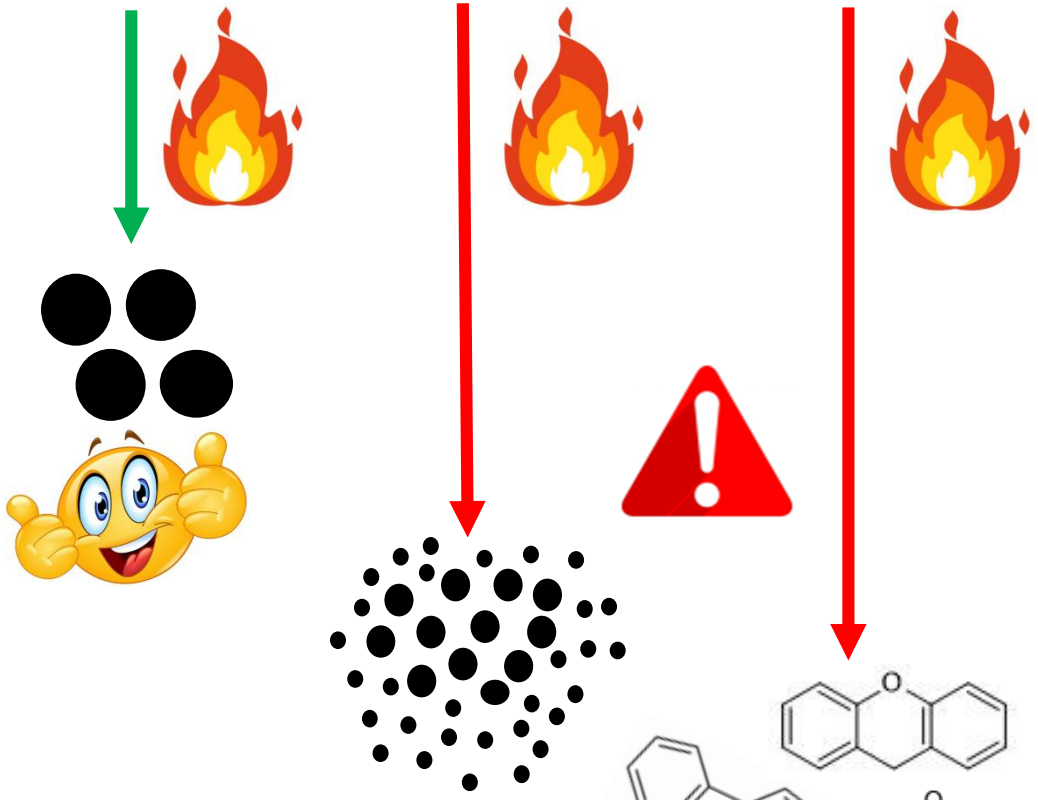
Context and Objective





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**?

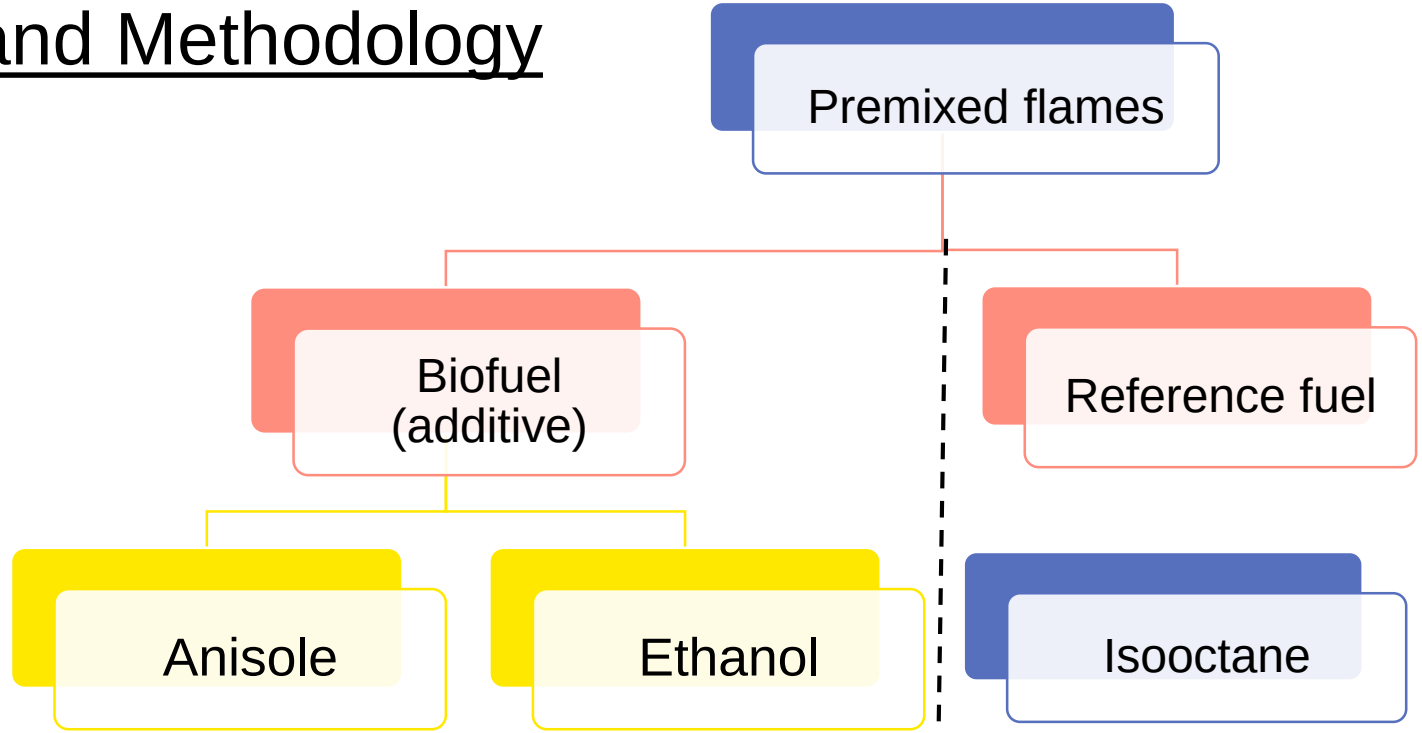
Approach and Methodology

- **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)



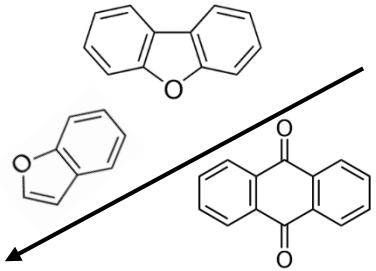
- Model molecules (can be obtained from biomass)
- They have a very rich chemistry
- Properties (potential automotive fuels)

a suitable substitute to represent a broad spectrum of real fuels

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

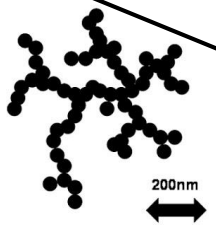
GC-SCION

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



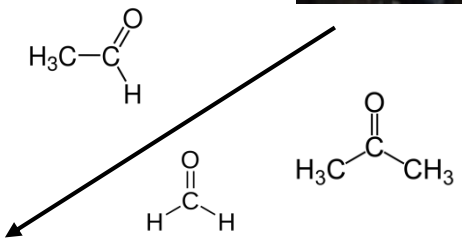
SMPS-1nm

- Scanning mobility Particle Sizer
- Can measure until 1 nm



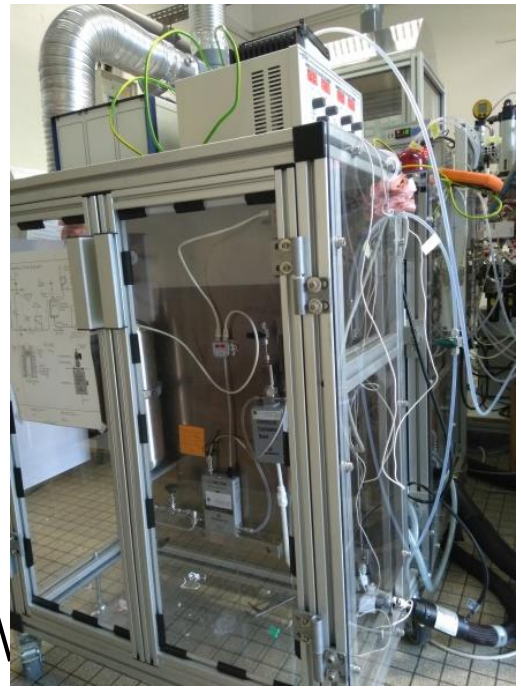
GC-Perkin

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

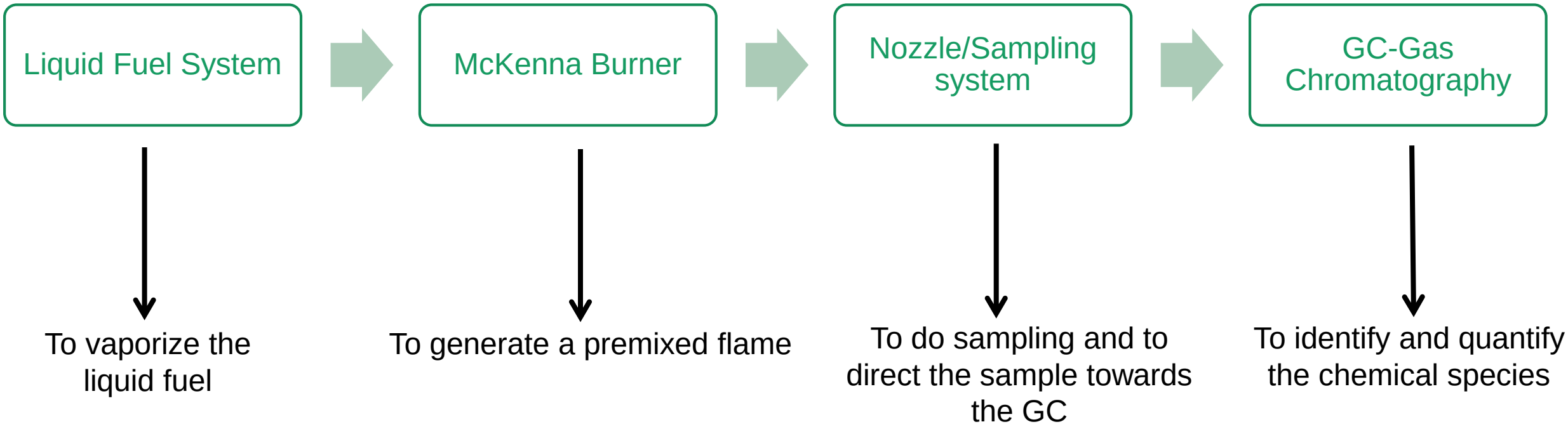


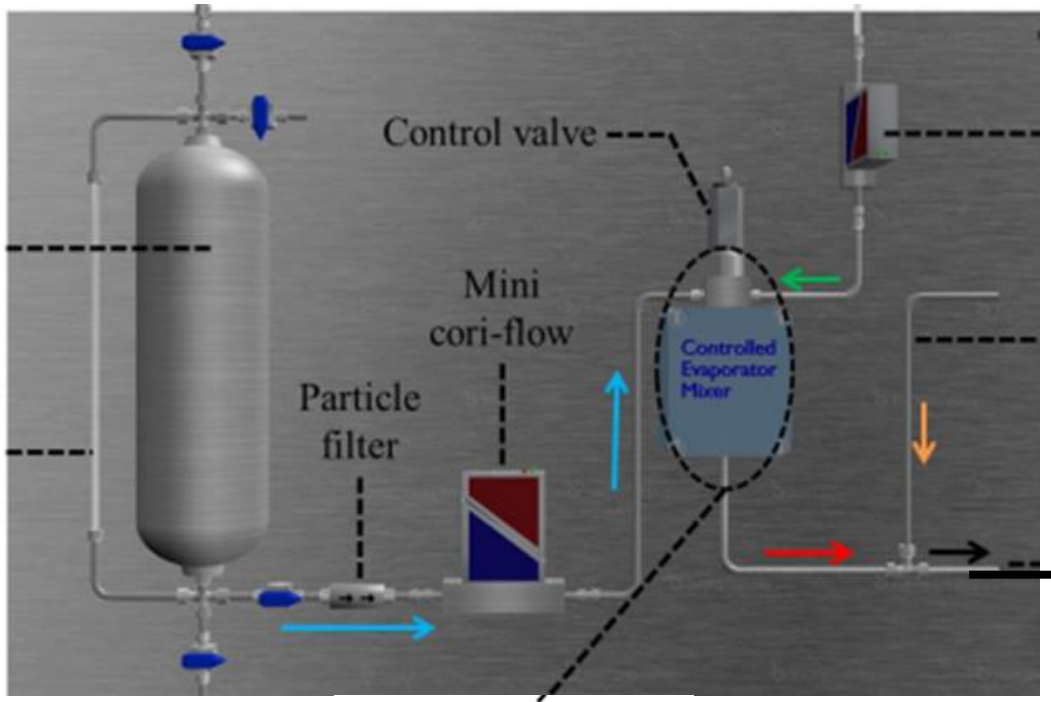
GC-MS Agilent

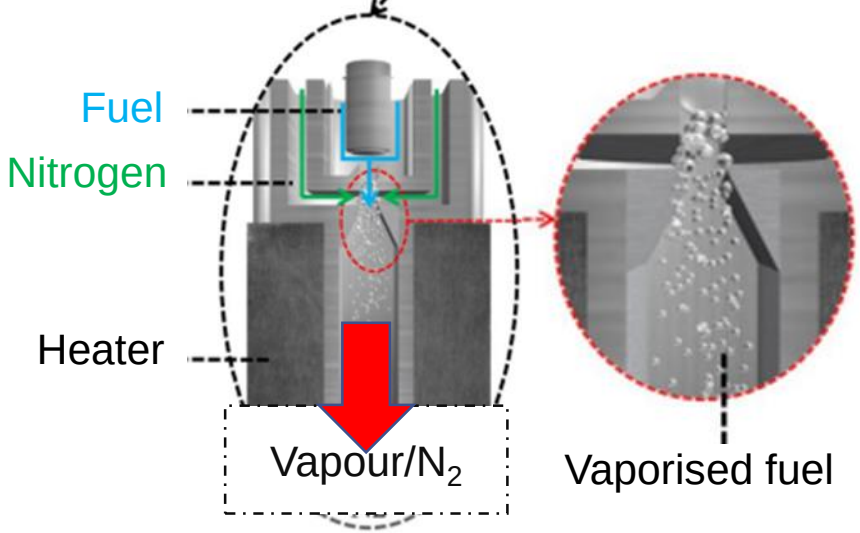
Experimental Room



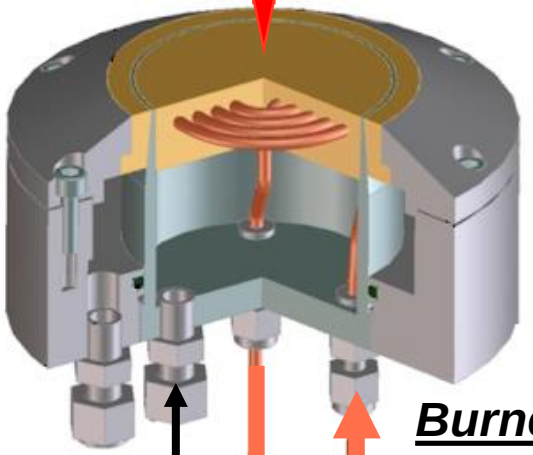
Global Scheme of the Flame-GC System





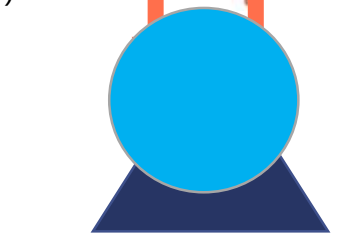


Nozzle



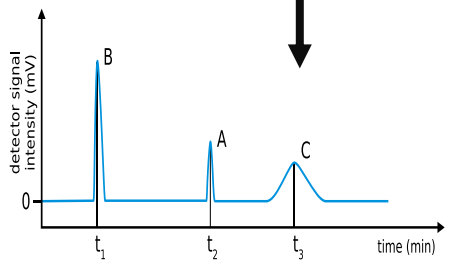
Burner

$Fuel+O_2+N_2$
(premixed)



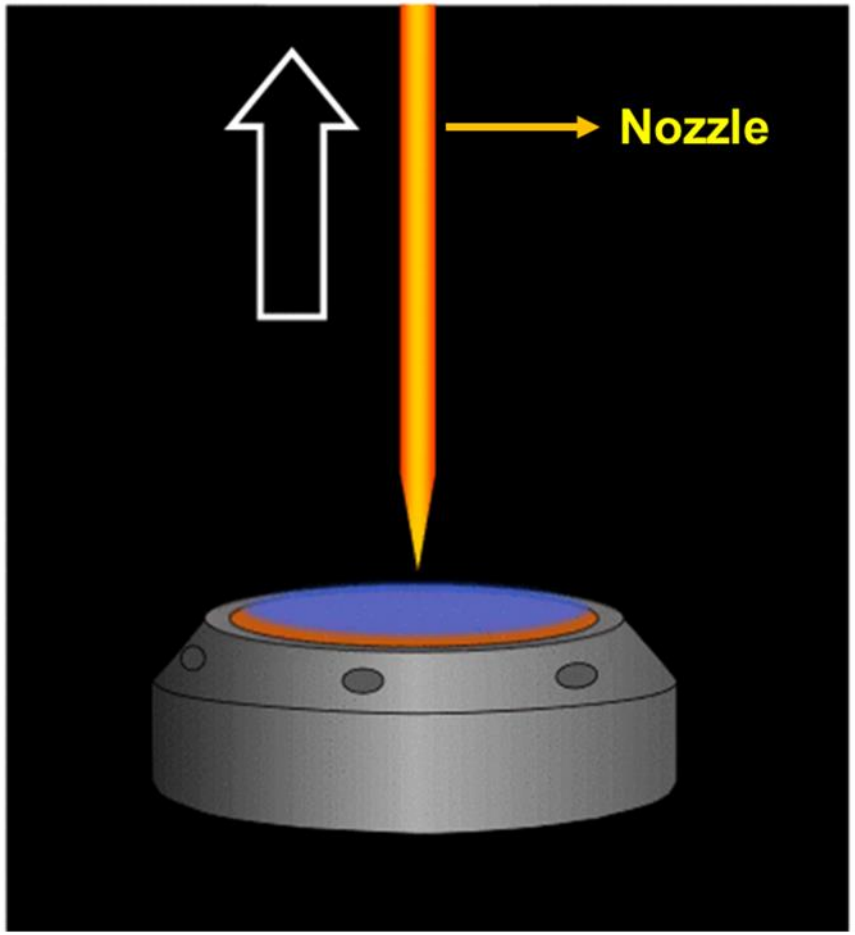
Circuit of cooling water

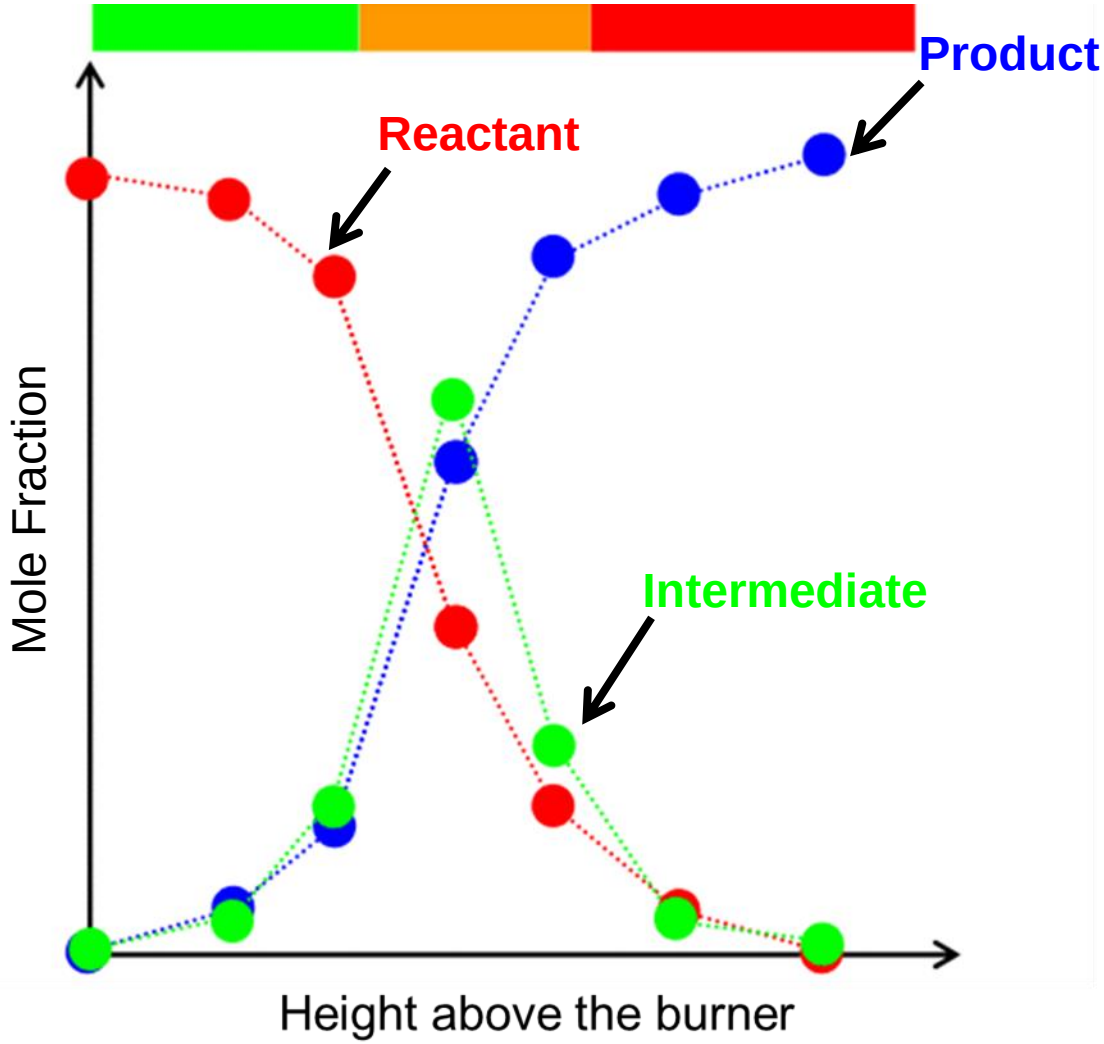
GC



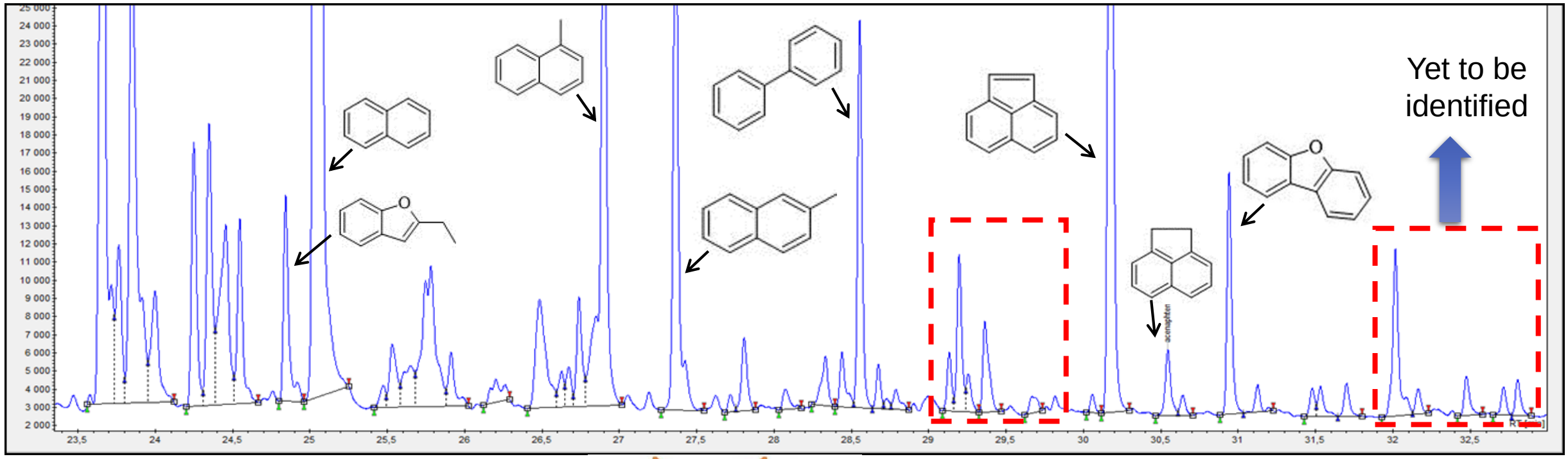
Liquid Fuel System

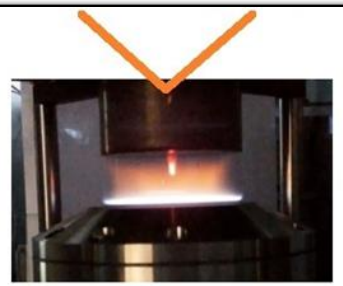
Sampling System



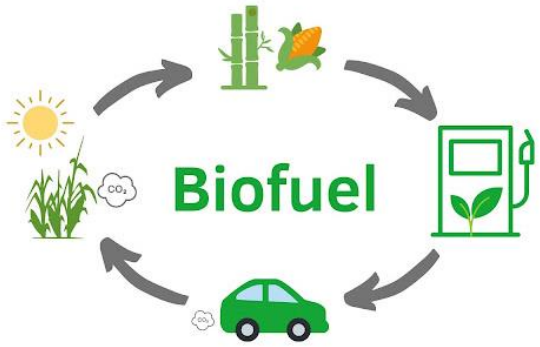


An example of a chromatogram …





Anisole flame (PC2A)



Flame Conditions

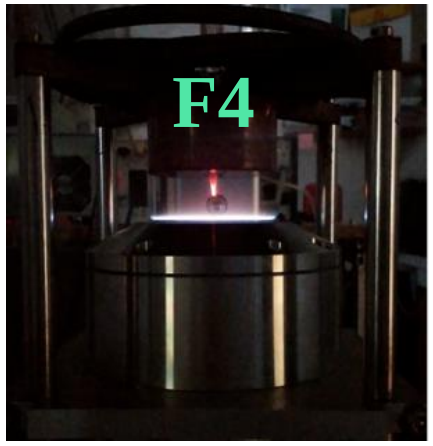
Series 1

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

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

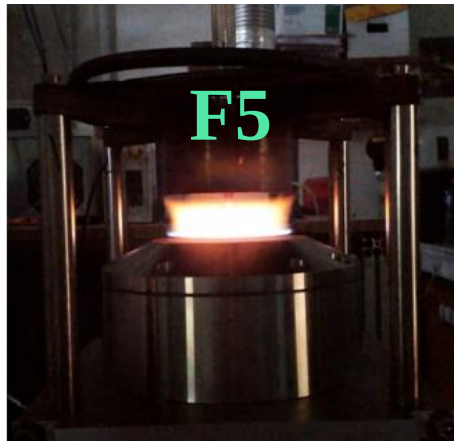
Equivalence Ratio = **1.82**
Anisole = **15%**

Series 2



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

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



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

Preliminary Results

1D GC Perkin

48 species

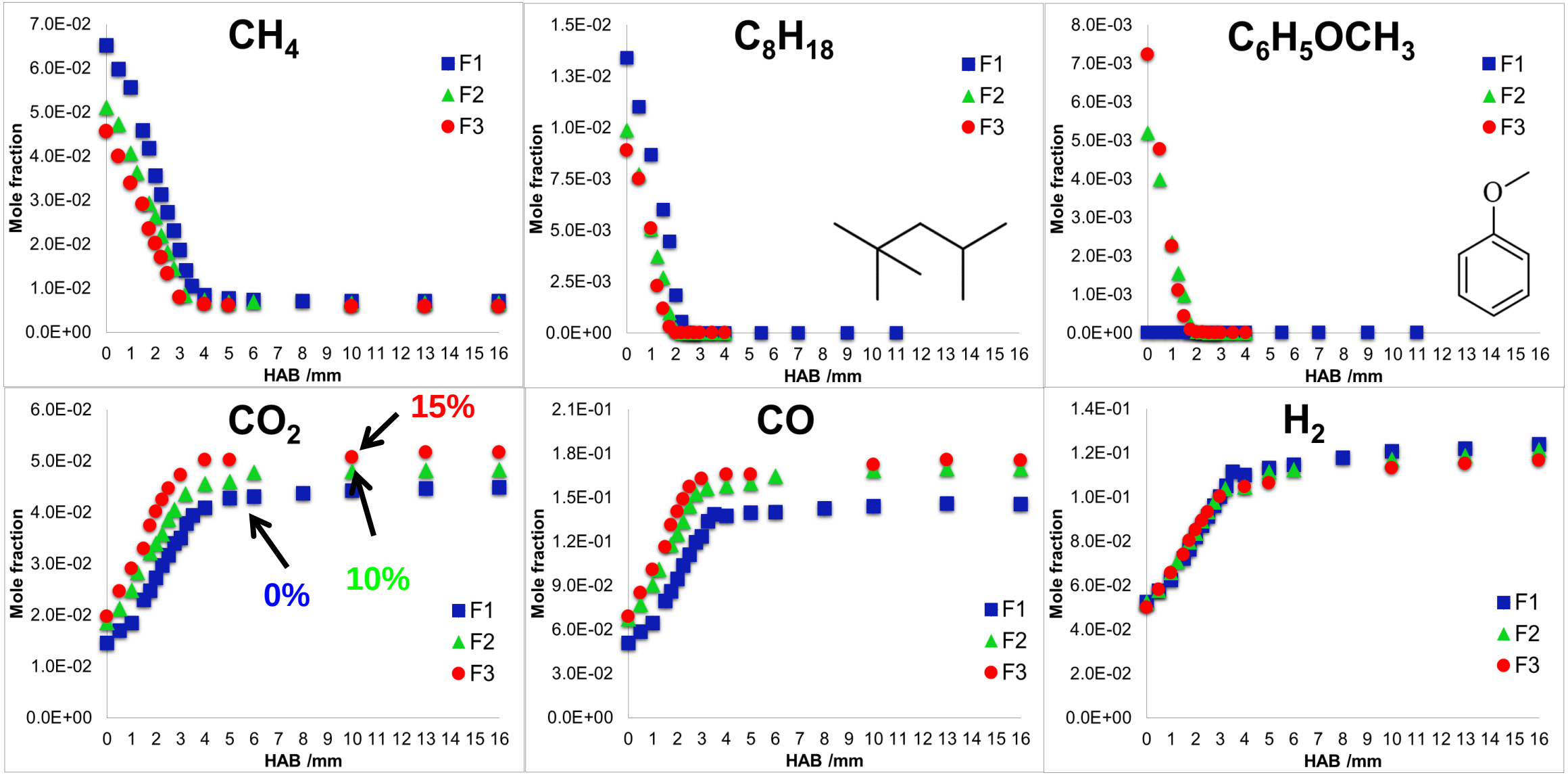
1D GC SCION

100 species

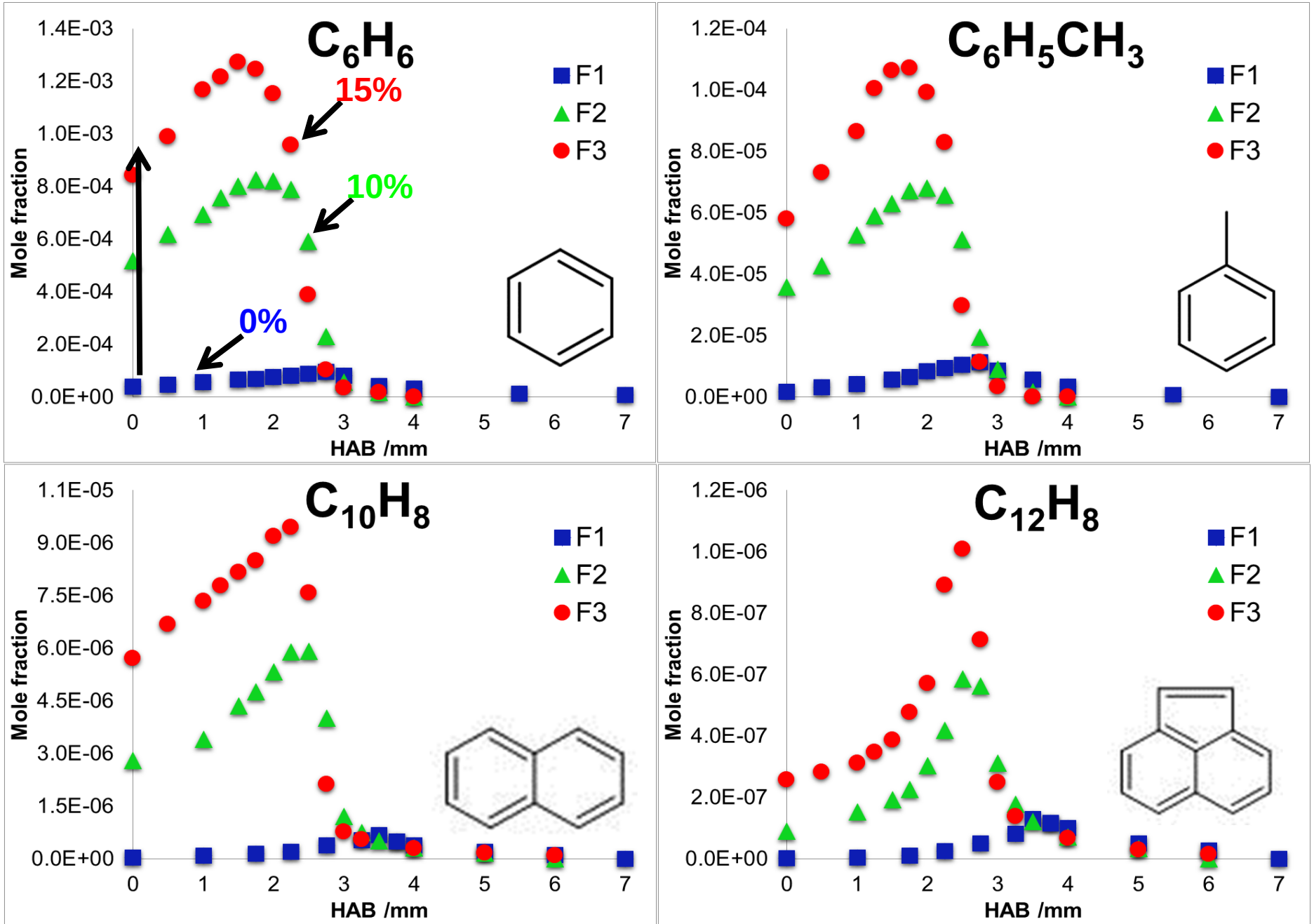
2D GC

Future work

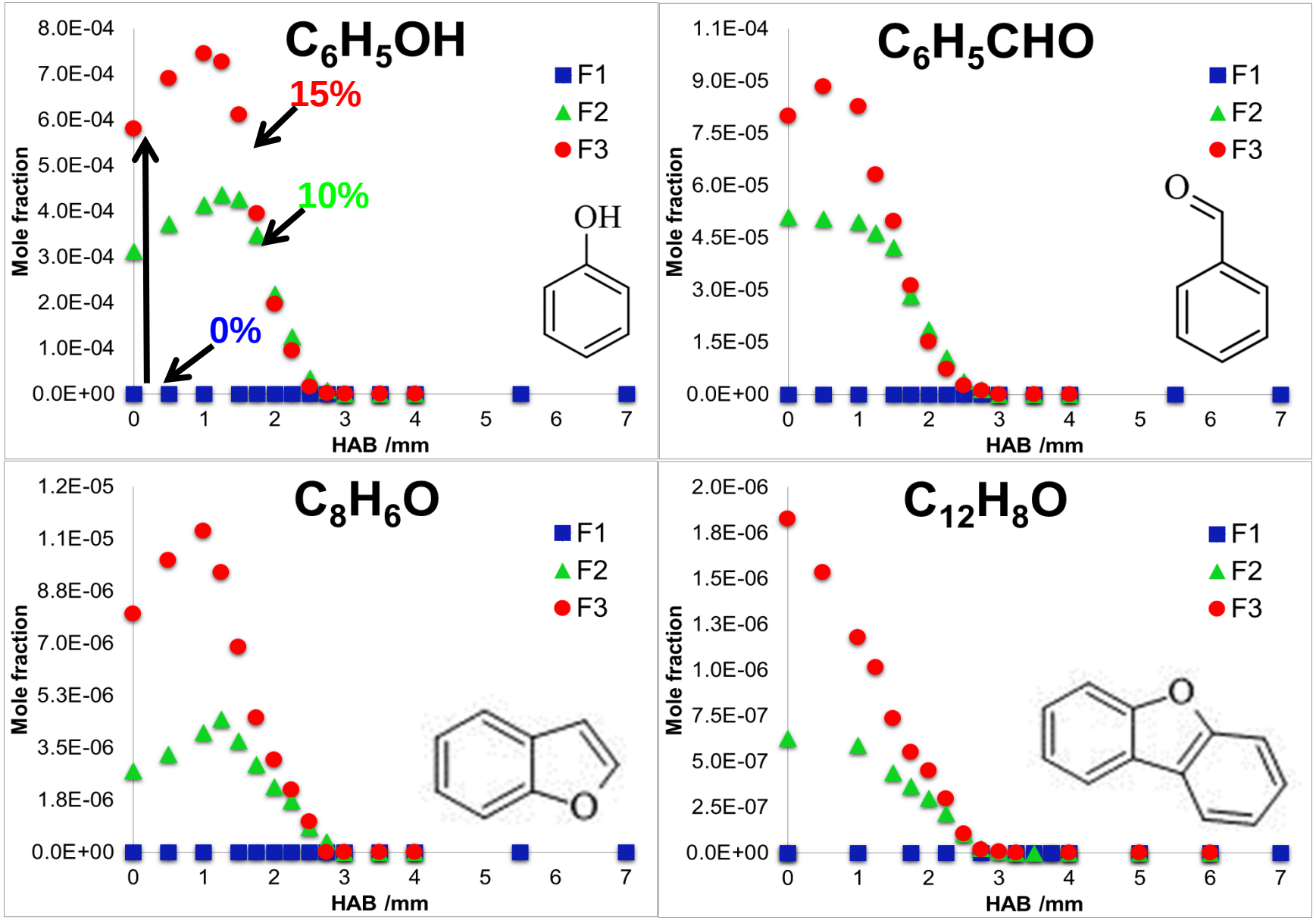
Selected Results: Series 1



Selected aromatics: Series 1

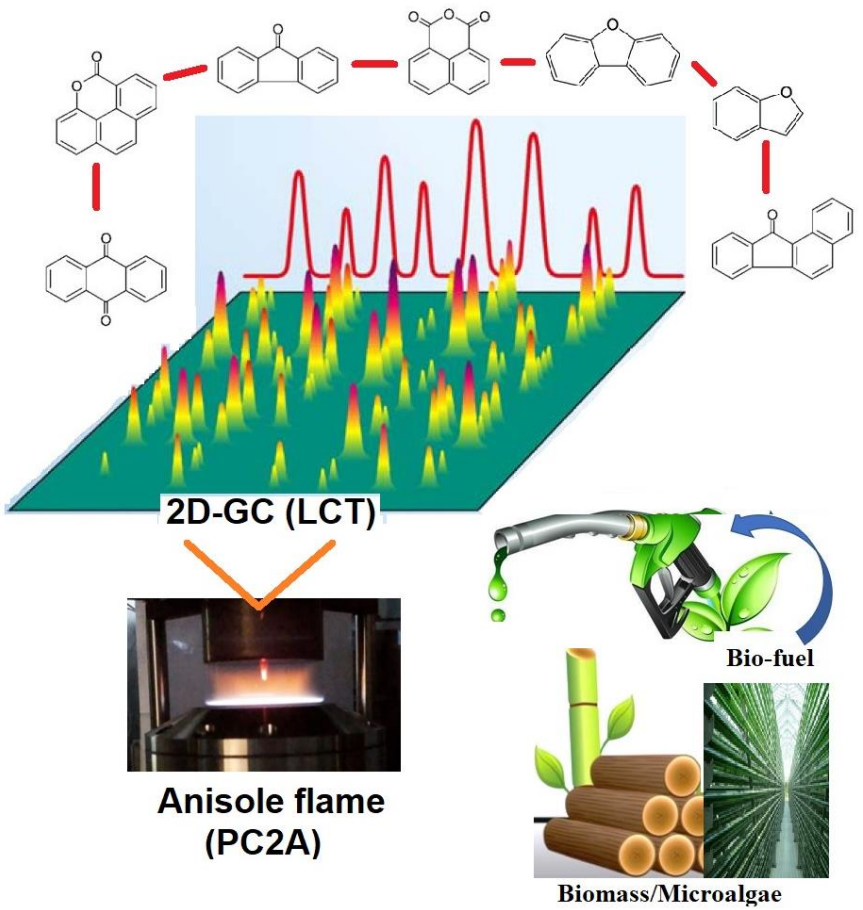


Selected oxy-aromatics: Series 1



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