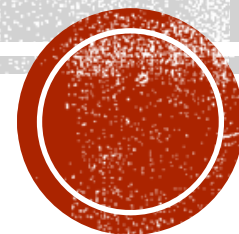


# Rosemary BIO Oil VS Rosemary Oil: Who Wins?



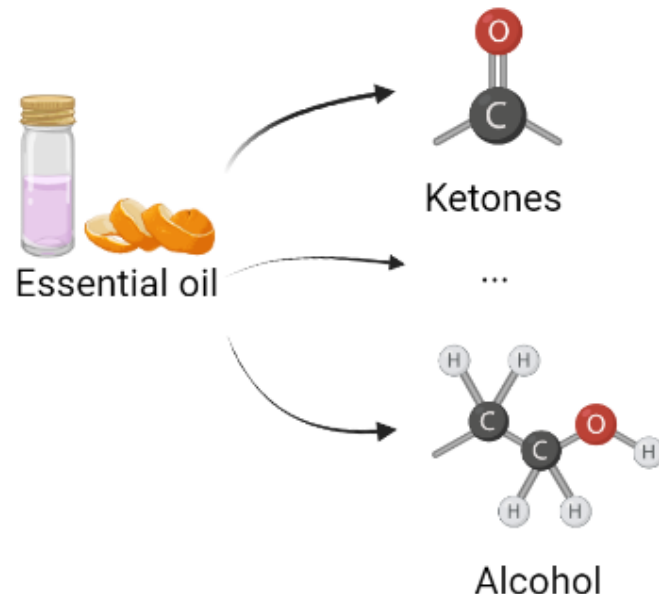
**Mónica Soeiro**, Mariana Louro,  
Marta Sousa Silva, Carlos Cordeiro

**End User School (Lille)**  
12<sup>th</sup>-16<sup>th</sup> December 2022

# Essential oil – Rosemary oil

Essential oils are obtained from various parts of the aromatic plants like flowers, peel, fruits, seeds, leaves, etc, origin by distillation or mechanical process from fruits like lemon or orange.

They are volatile liquids with high solubility in alcohol or ether and low solubility in water. Usually colourless, present a characteristic odour and are complex mixtures composed by different functional group like aldehydes, alcohols, ketones and organic acids



## Rosemary oil (*Rosmarinus officinalis* L.)

Due to the antibacterial and antioxidant properties, the rosemary oil is used in food cosmetics and perfume industries.

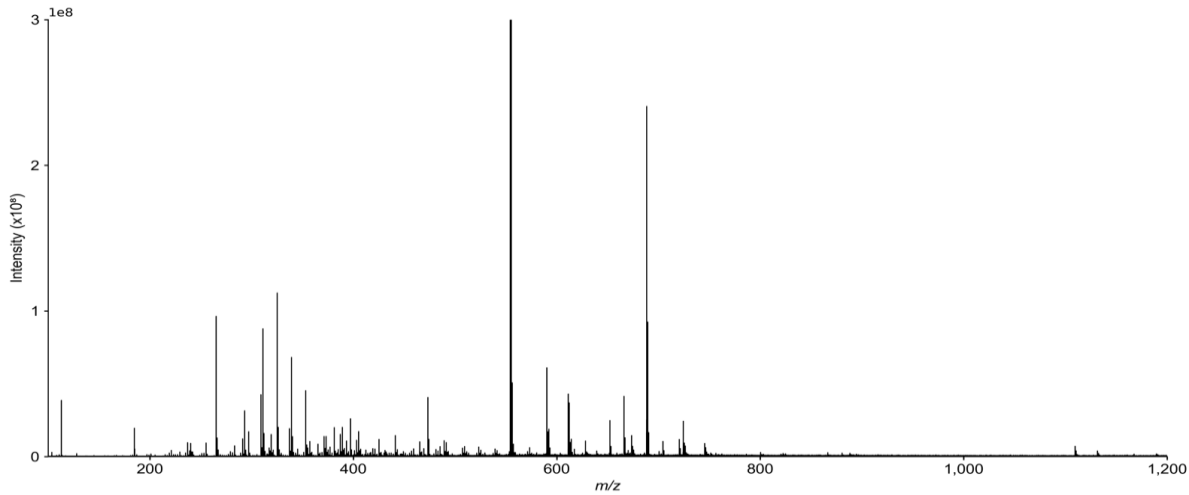
Rosemary oil

Rosemary oil (BIO)

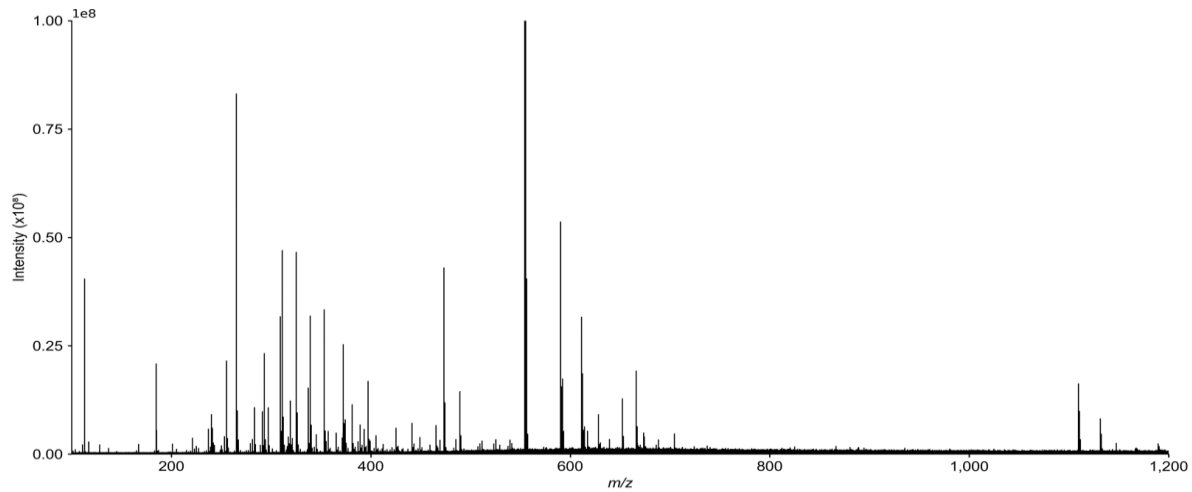
# Mass Spectrometry – Data Analysis

Negative mode

Rosemary

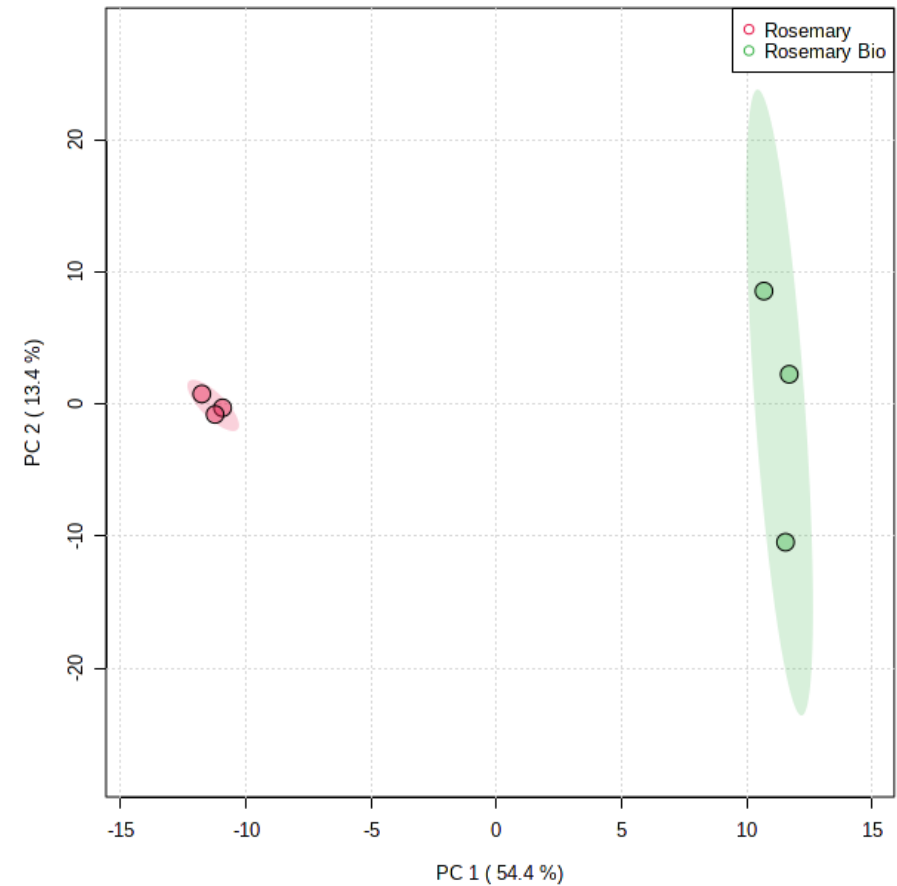


Rosemary Bio



PCA

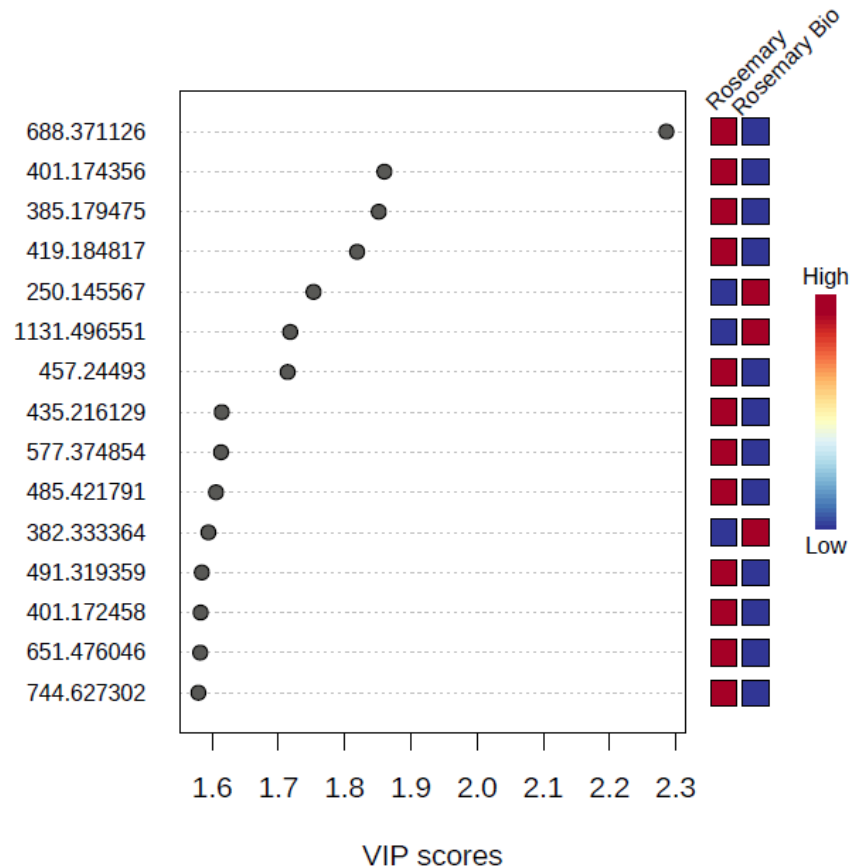
Scores Plot



# Mass Spectrometry – Data Analysis

Negative mode

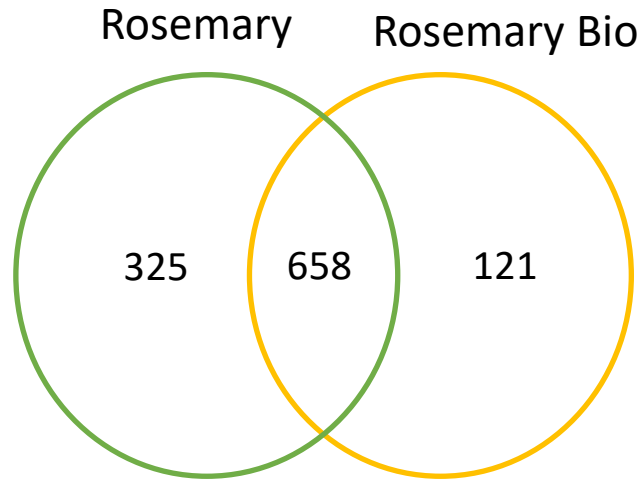
PLS-DA



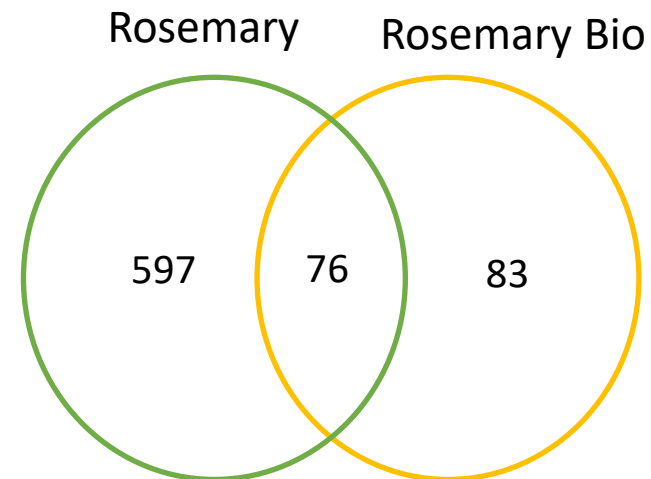
m/z	MW (Da)	Compound Name
688.37113	689.37827	-
401.17436	402.18163	-
385.17948	386.18675	-
419.18482	384.21545	-
250.14557	251.15284	-
1131.49655	1132.50383	-
457.24493	458.25221	-
435.21613	436.22341	-
577.37485	578.38213	Asparagoside A
485.42179	486.42907	-
382.33336	383.34064	-
491.31936	492.32664	-
401.17246	402.17973	Dibenzo-P-dioxina
651.47605	652.48332	-
744.62730	745.63458	-

# Mass Spectrometry – Data Analysis

## Negative mode



## Positive mode



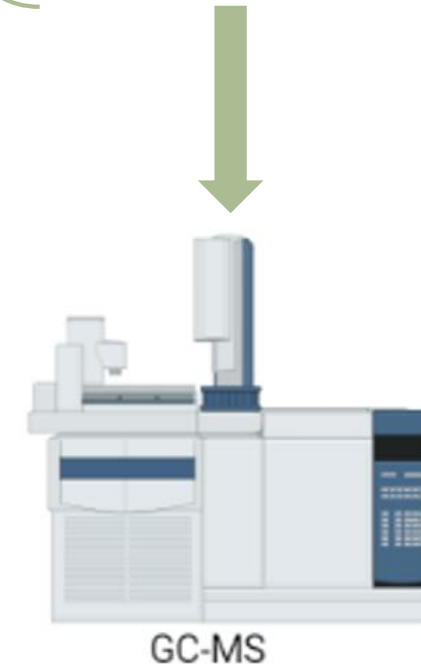
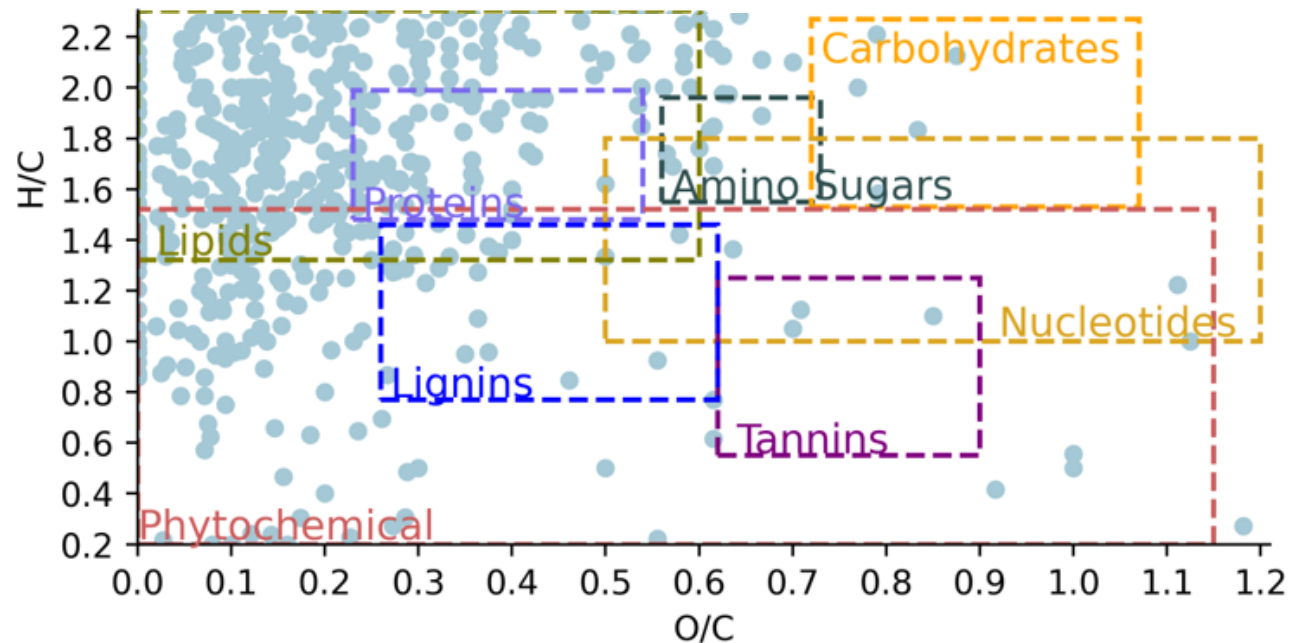
# Mass Spectrometry – Data Analysis

Negative mode

Van Krevelen Diagram

Fatty Acids

- ❖ Palmitic acid
- ❖ Stearic acid
- ❖ Oleic acid
- ❖ Linoleic acid
- ❖ Pentadecanoic acid
- ❖ Heptadecanoic acid

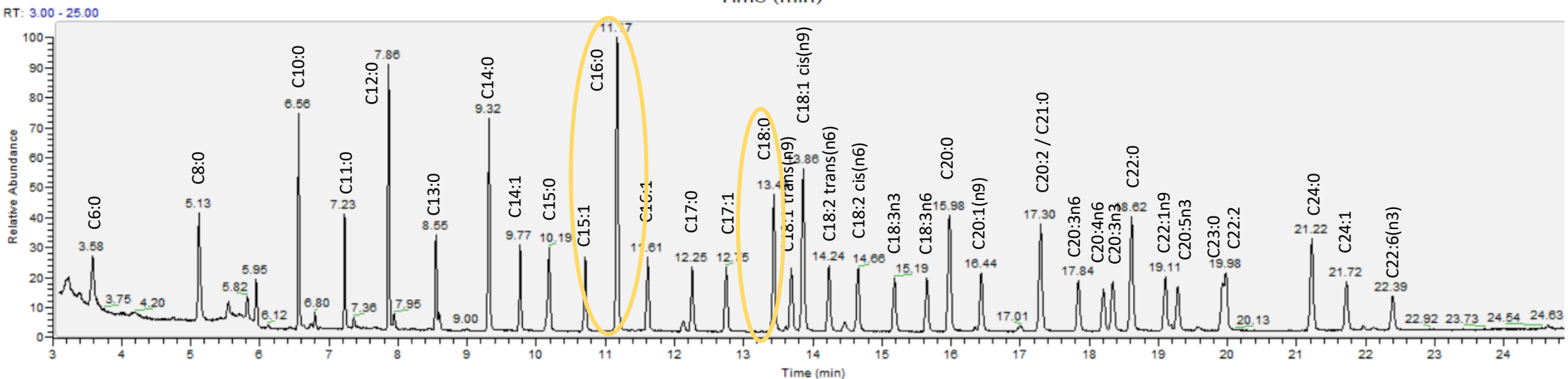
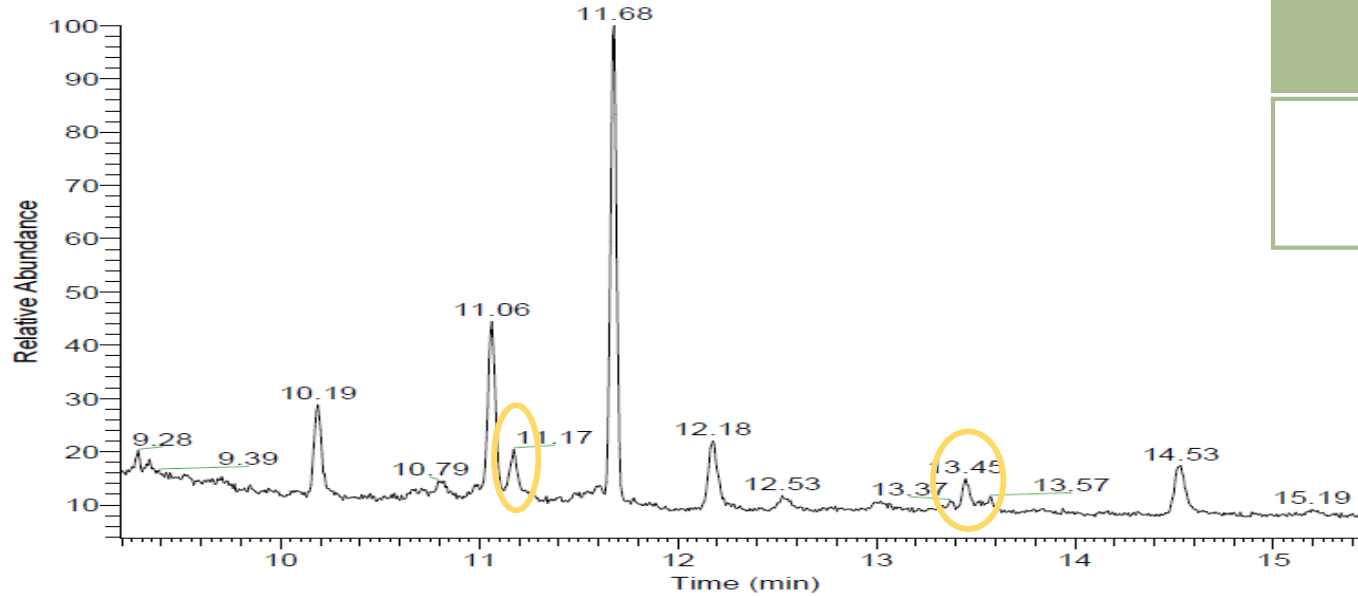


# Mass Spectrometry – GC-MS

Rosemary Bio oil  
(*Rosmarinus officinalis* L.)

Palmitic acid (PA)  
Stearic acid (SA)

$C_{PA} = 0.324$  mg/ml  
 $C_{SA} = 0.027$  mg/ml



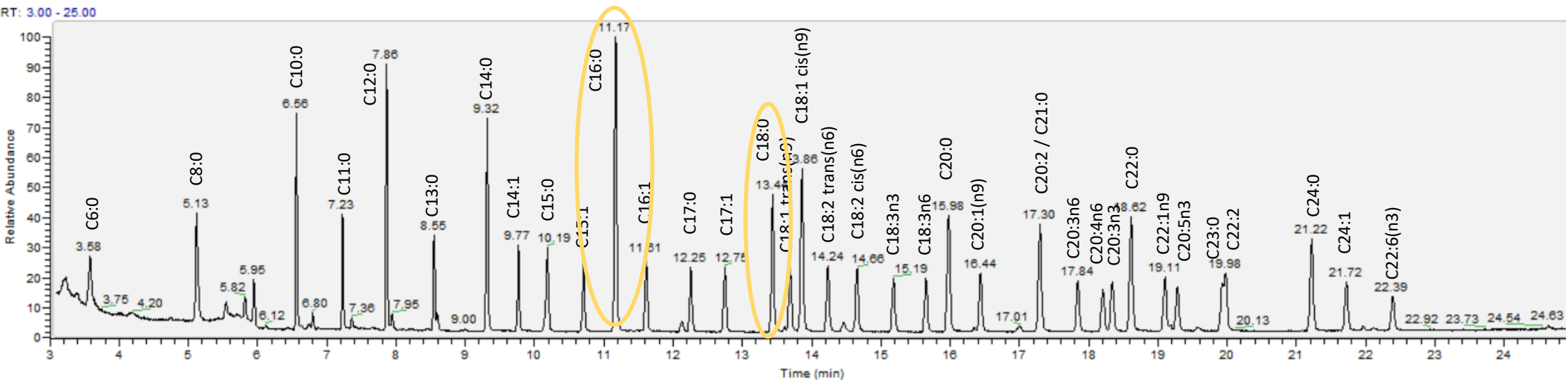
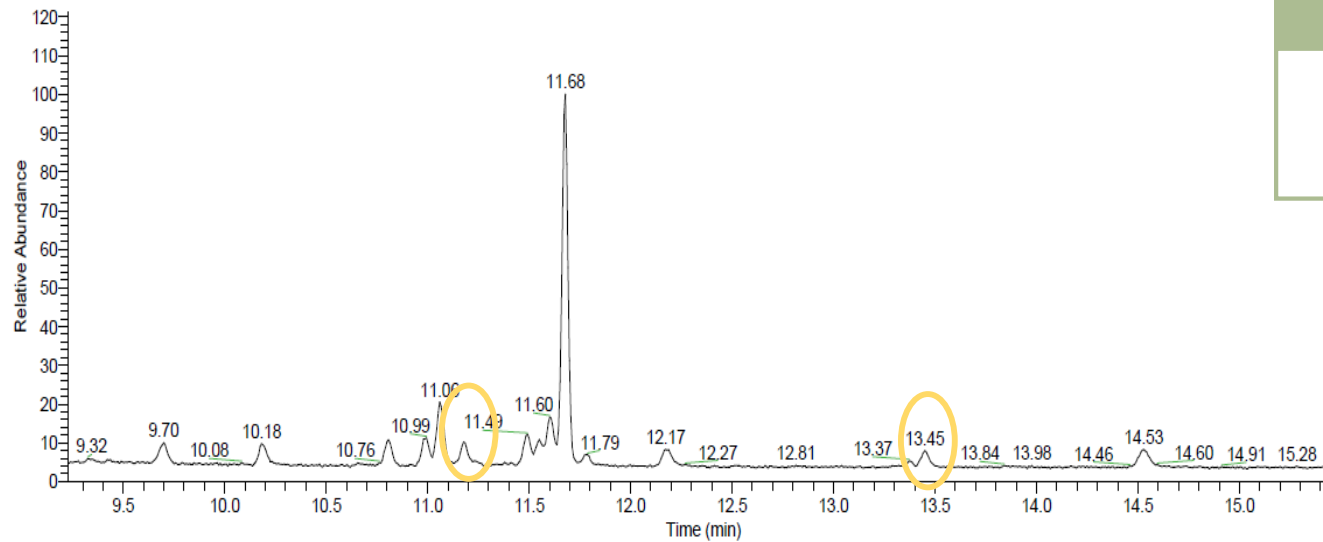
# Mass Spectrometry – GC-MS

Rosemary oil  
(*Rosmarinus officinalis* L.)

Palmitic acid (PA)  
Stearic acid (SA)

$C_{PA} = 0.321$  mg/ml

$C_{SA} = 0.027$  mg/ml





# Conclusion

- ❖ It is possible to distinguish rosemary oil from rosemary BIO oil through the identified peaks or compounds
- ❖ It is possible to conclude that the existence of fatty acids in negative mode is confirmed in the analysis of the FT-ICR-MS
- ❖ It is possible to identify and quantify fatty acids compounds by GC-MS

# Future Perspectives

- ❖ Analyze and identify other compounds of interest in the FT-ICR-MS
- ❖ Analyze other types of essential oils of interest for food industry

# Acknowledgment



Ciências  
ULisboa

FT-ICR-SMS-Lab

