

**Sviluppo di modelli di classificazione di relazione
composizione-attività di tipo quantitativo (QCAR) con
algoritmi di Machine Learning e valutazione dell'attività
antibatterica di una serie di componenti di oli
essenziali nei confronti di *Klebsiella Pneumoniae*
multi-antibiotico resistente.**



SAPIENZA
UNIVERSITÀ DI ROMA

**Facoltà di Farmacia e Medicina
Corso di Laurea in Biotecnologie
Farmaceutiche
Tesi sperimentale in Chimica Farmaceutica
a.a 2022/2023**

Laureanda: Arnaut Marcela
Matricola: 1679130

Relatore: Prof. Rino Ragno
Correlatore: Dott.ssa Alessandra Oliva



Introduzione



Welcome AI4EssOil			
Stats			
2756	1107	1243	20950
Extracts compositions	Plants	Publications analysed	Biological activities stored

OLI ESSENZIALI



DATA CLEANING



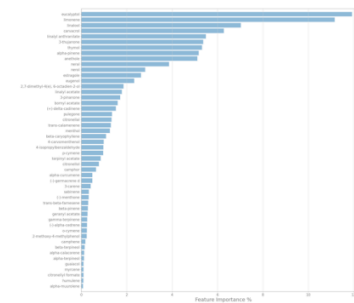
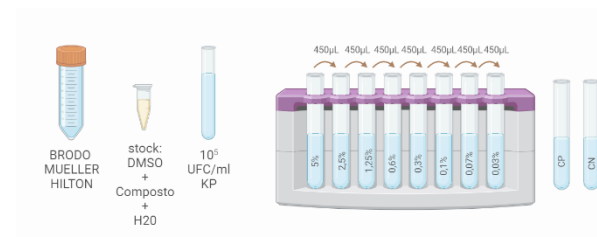
MODELLIZZAZIONE

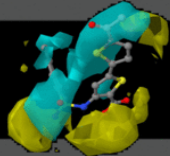


ANALISI



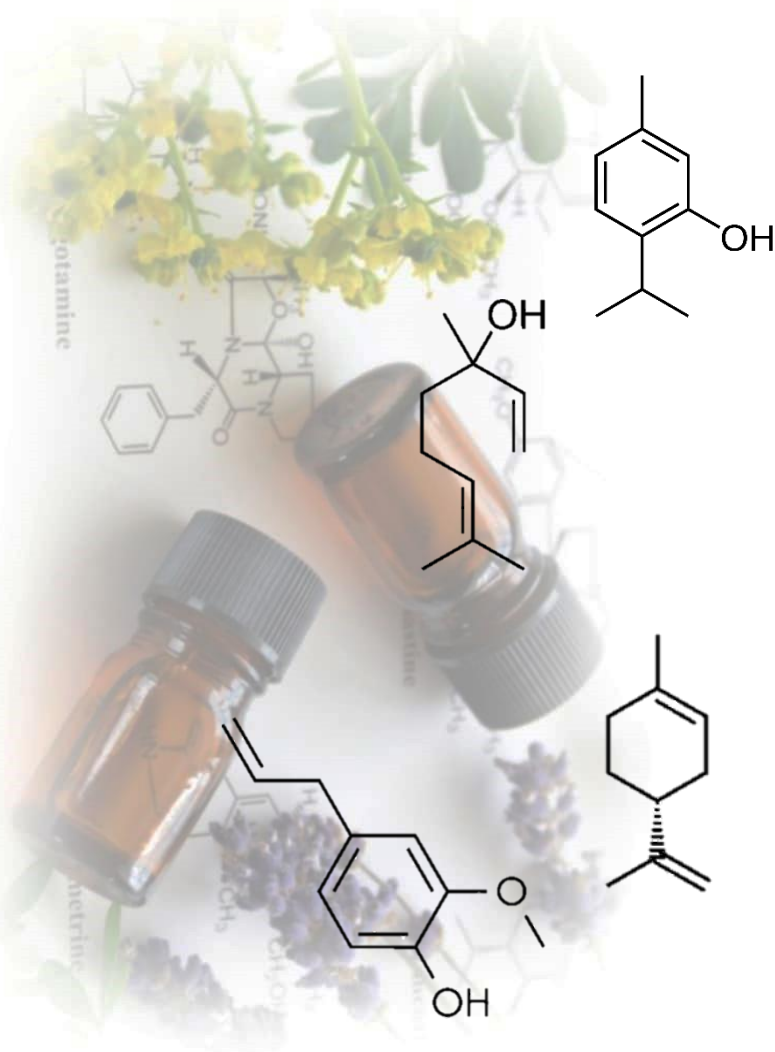
SAGGI MICROBIOLOGICI

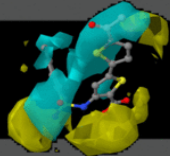




OLI ESSENZIALI

- Sostanze liquide, oleose, volatili e con un odore aromatico.
- Miscela di composti complessi.
- Attività farmacologica e tossicologica: attribuita ad innumerevoli gruppi funzionali.
- Agevolare la ricerca di un olio essenziale “*ex novo*” o progettarlo.





Introduzione

OLI ESSENZIALI



DATA CLEANING



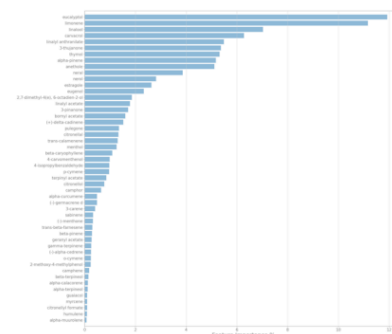
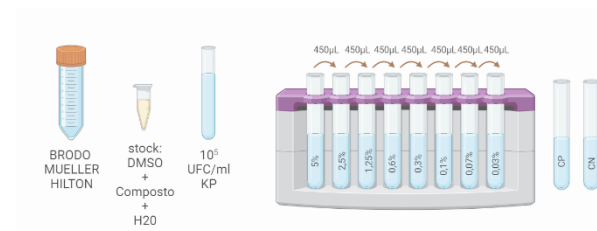
MODELLIZZAZIONE



ANALISI

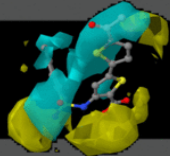


SAGGI
MICROBIOLOGICI

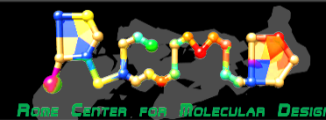


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DATA CLEANING



Welcome AI4EssOil

Stats

2756

1107

1243

20950

Extracts
compositions

Plants

Publications
analysed

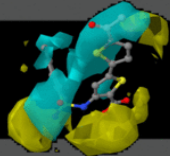
Biological activities
stored

DATASET I: 61 oli essenziali e 224 componenti, *Klebsiella Pneumoniae* **resistente** ai carbapenemi.

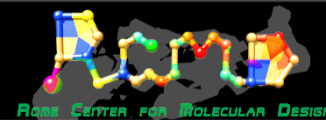


DATASET II: 149 oli essenziali e 816 componenti, *Klebsiella Pneumoniae* **sensibile** ai carbapenemi.

<https://www.ai4essoil.com/front/>



DATA CLEANING



Welcome AI4EssOil

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2756	1107	1243	20950
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<https://www.ai4essoil.com/front/>

DATA CLEANING



DATASET I: 61 oli essenziali e
224 componenti, *Klebsiella
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e 816 componenti, *Klebsiella
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Introduzione

OLI ESSENZIALI



DATA CLEANING



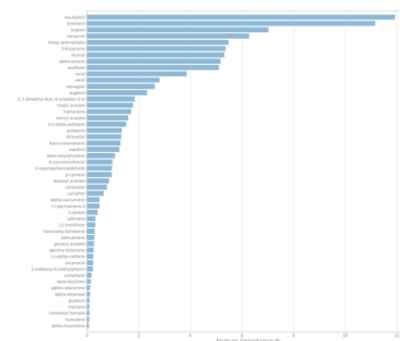
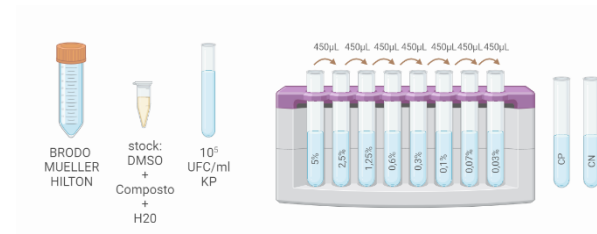
MODELLIZZAZIONE



ANALISI



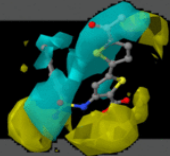
SAGGI
MICROBIOLOGICI



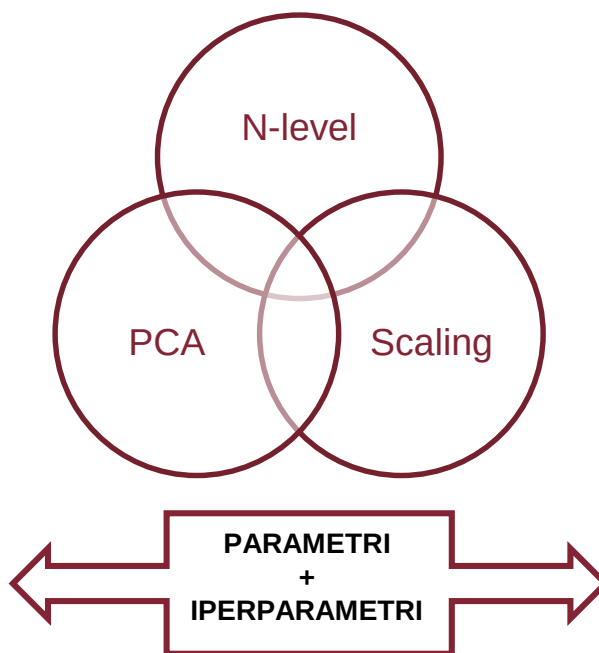
Welcome AI4EssOil

Stats

Extracts compositions	Plants	Publications analysed	Biological activities stored
2756	1107	1243	20950



MODELLIZZAZIONE

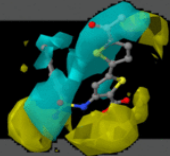


ALGORITMI:

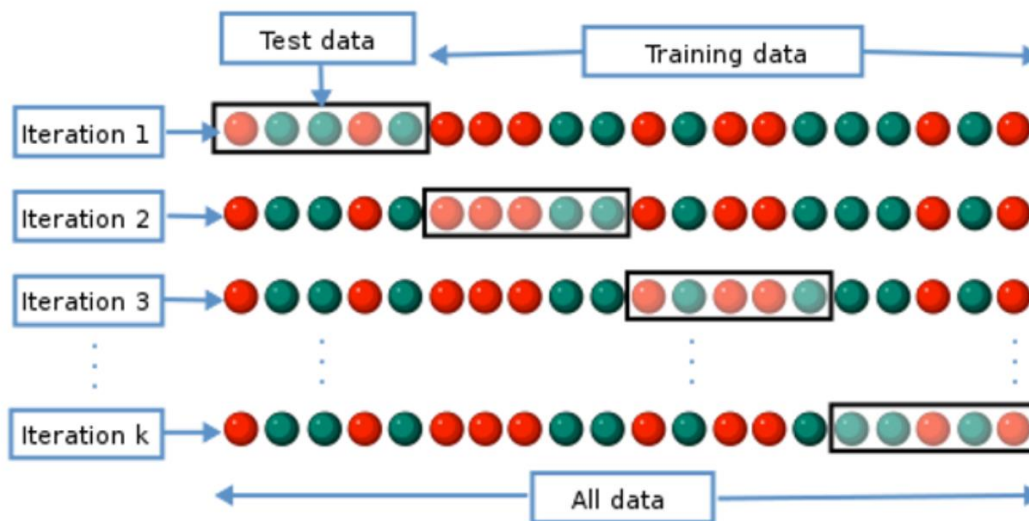
- SVM
- Random forest
- Gradient boosting
- K-NN
- Decision Tree

ITERAZIONI:

- 100
- 1000
- 10000
- 100000

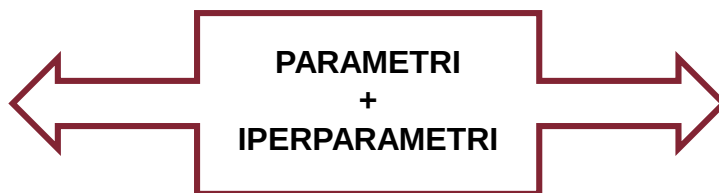


MODELLIZZAZIONE



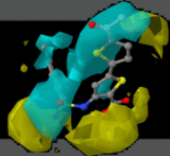
ALGORITMI:

- SVM
- Random forest
- Gradient boosting
- K-NN
- Decision Tree



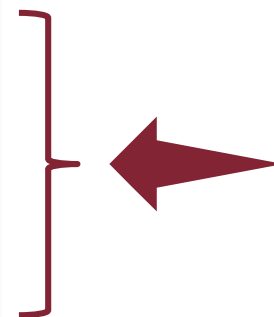
ITERAZIONI:

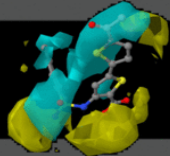
- 100
- 1000
- 10000
- 100000



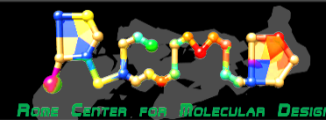
MODELIZZAZIONE: I DATASET

THRESHOLD MIC = 0,216%v/v-> ATTIVI: 18 NON ATTIVI:43	
CLASSIFICATORE	SVM
N° LIVELLI	2
SCALING	FALSE
PCA	0
MCC_PRED	0,803
MCC_CV	0,559
MCC_FIT	0,921

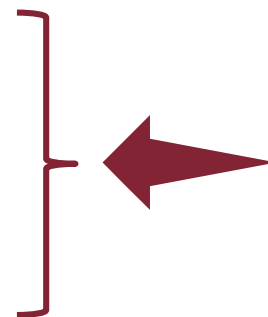


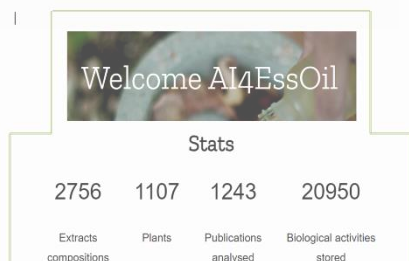
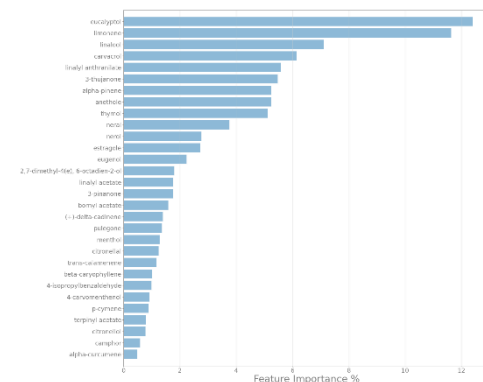
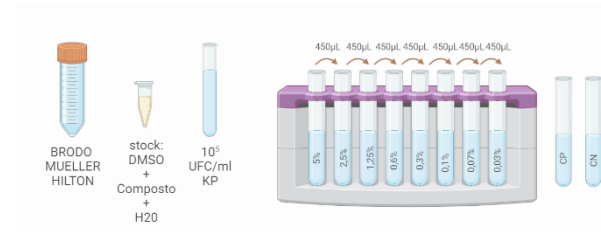
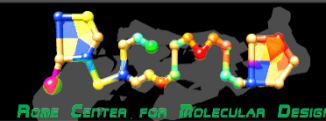


MODELIZZAZIONE: II DATASET



THRESHOLD MIC = 0,057%v/v-> ATTIVI: 76 NON ATTIVI:73	
CLASSIFICATORE	GB
N° LIVELLI	3
SCALING	TRUE
PCA	0,7
MCC_PRED	0,519
MCC_CV	0,341
MCC_FIT	0,880



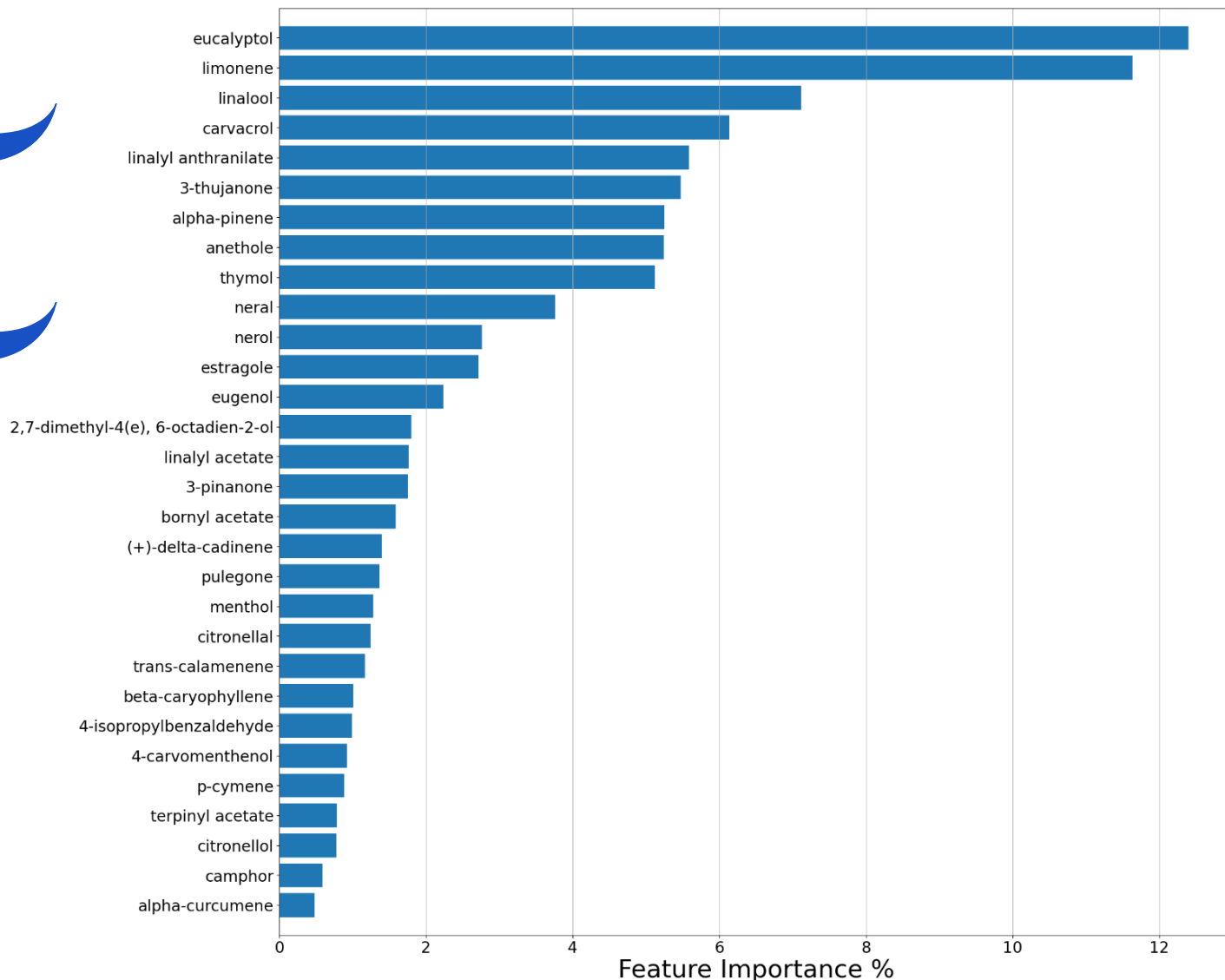


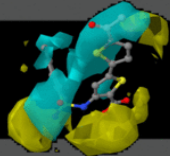


ANALISI SKATER: MIC I DATASET

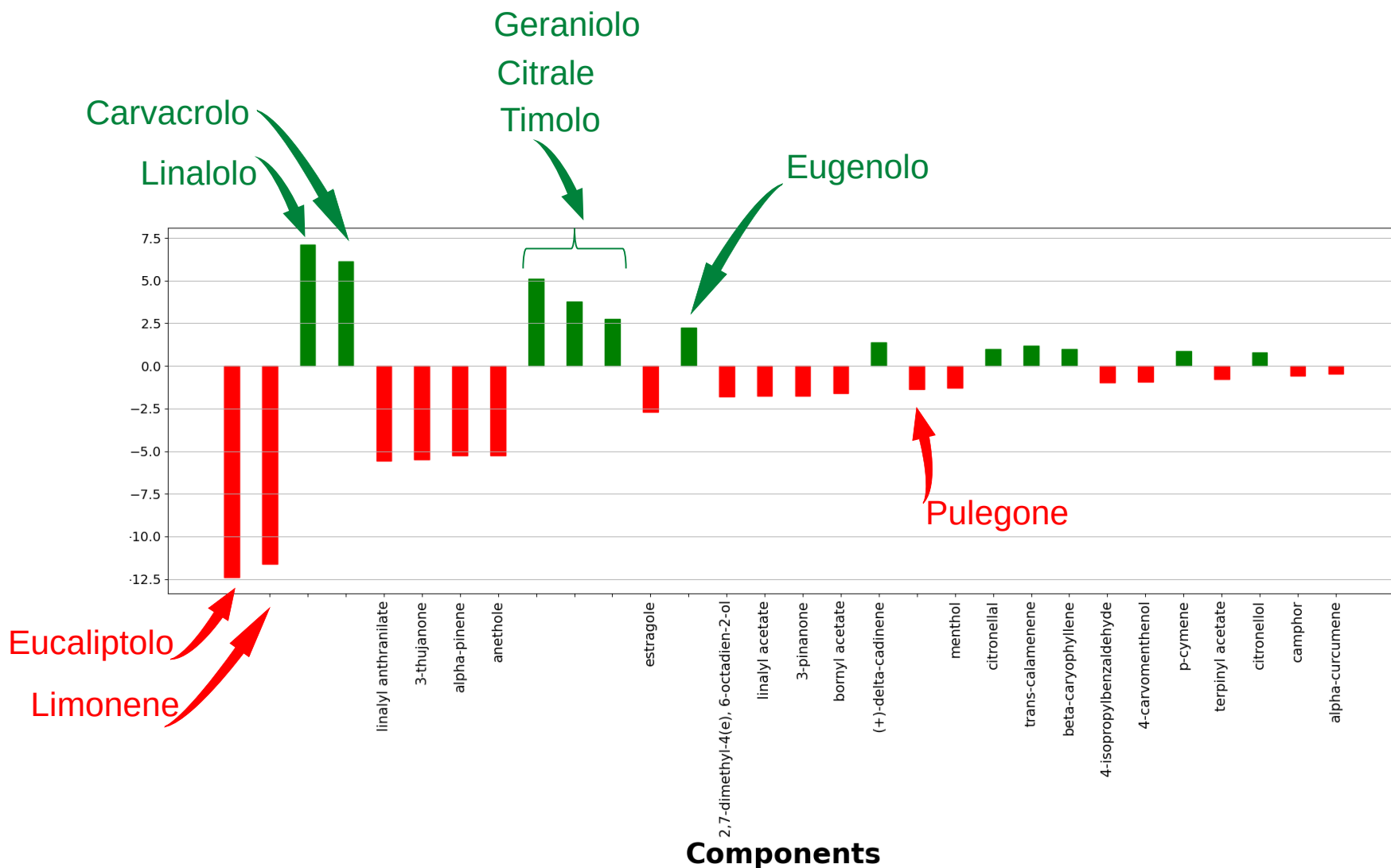
Eucaliptolo
Limonene
Linalolo
Carvacrolo

Timolo
Citrale
Geraniolo
Eugenolo





Features Importance PESATA: I DATASET





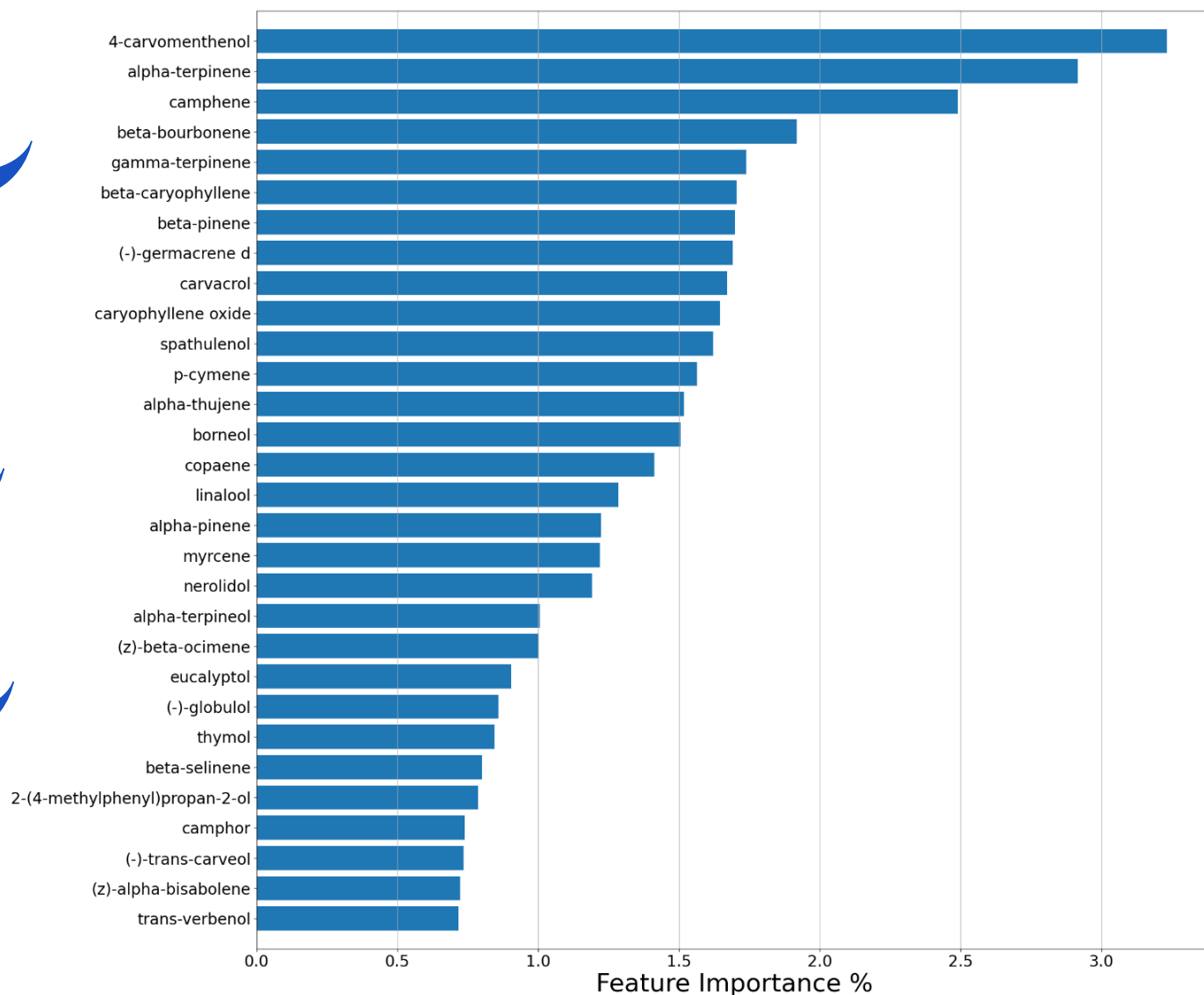
ANALISI SKATER: MIC II DATASET

4-carvomentenolo
Gamma-terpinene

Beta-cariofillene
Carvacrolo

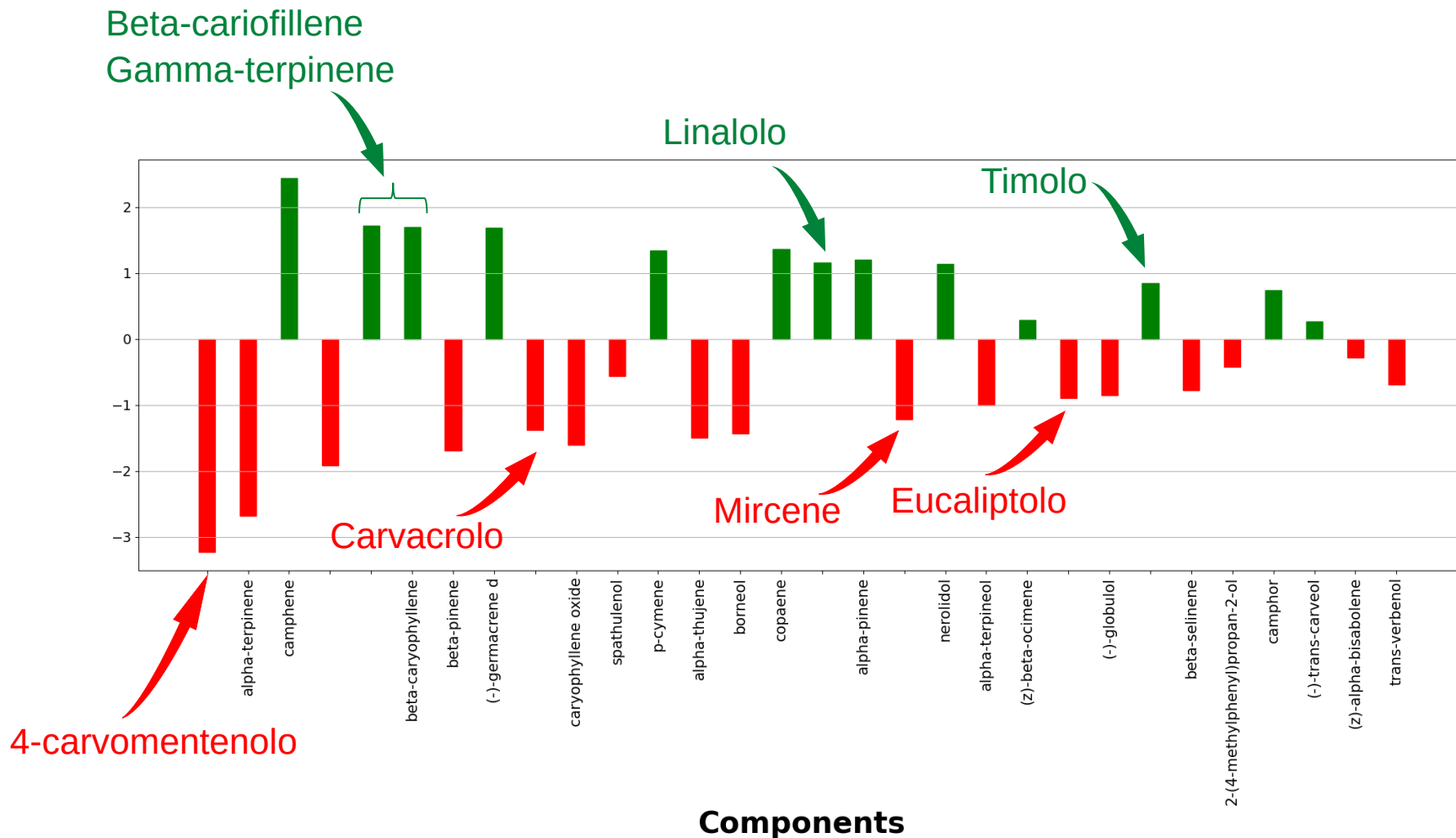
Linalolo

Eucaliptolo
Timolo





Features Importance PESATA : II DATASET





Introduzione

OLI ESSENZIALI



DATA CLEANING



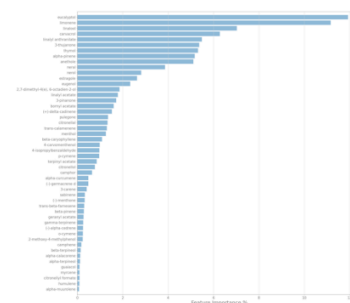
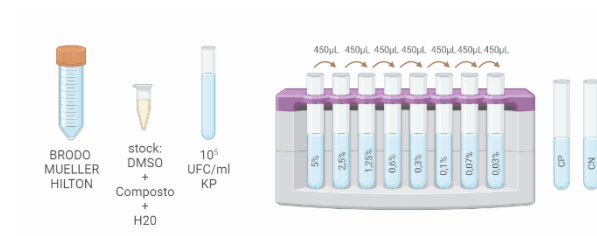
MODELLIZZAZIONE



ANALISI



**SAGGI
MICROBIOLOGICI**



Welcome AI4EssOil

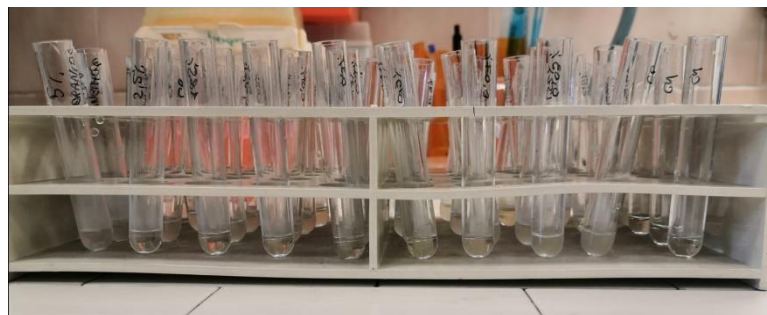
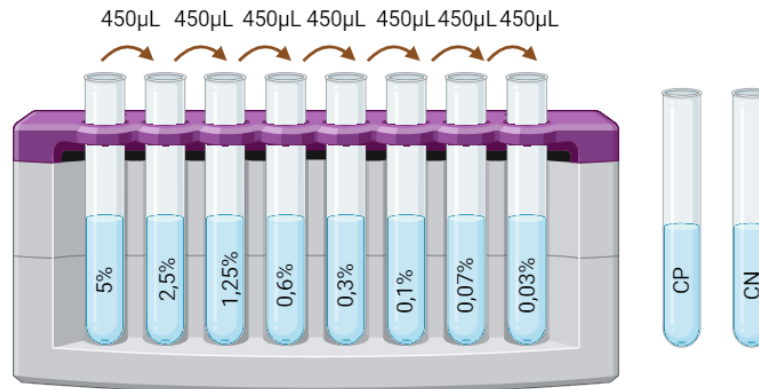
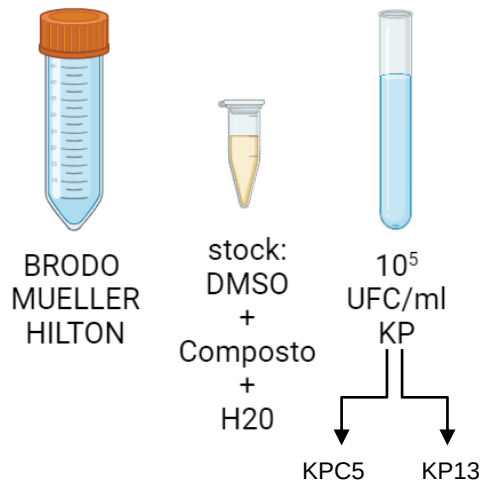
Stats

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Extracts compositions Plants Publications analysed Biological activities stored

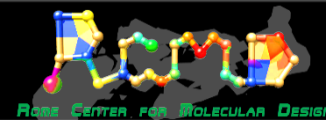


SAGGI MICROBIOLOGICI

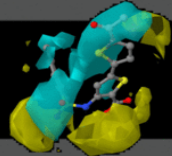




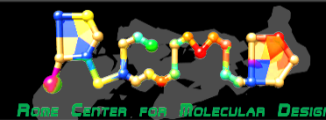
SAGGI MICROBIOLOGICI: I DATASET



NOME COMPOSTO	KLEBSIELLA PNEUMONIAE resistente ai carbapenemi
	MIC
Linalolo	0,6%
Limonene	0,6%
Eucaliptolo	5%
alfa-pinene	>5%
Carvacrolo	$\leq 0,03\%$
Timolo	$\leq 0,03\%$
p-cimene	>5%
Citronellal	5%
Eugenolo	$\leq 0,03\%$
Mentolo	0,07%
Acetato di linalile	>5%
Citrale	0,07%
Pulegone	2,5%
Anetole	>5%
Geraniolo	0,07%
beta-cariofillene	>5%



SAGGI MICROBIOLOGICI: II DATASET



NOME COMPOSTO	KLEBSIELLA PNEUMONIAE sensibile ai carbapenemi
	MIC
Linalolo	$\leq 0,03\%$
Limonene	0,6%
Eucaliptolo	5%
alfa-pinene	>5%
Carvacrolo	$\leq 0,03\%$
Timolo	$\leq 0,03\%$
p-cimene	>5%
alfa-fellandrene	2,5%
4-carvomentenolo	$\leq 0,03\%$
gamma-terpinene	5%
Mircene	>5%
beta-pinene	>5%
Terpinolene	5%
beta-cariofillene	>5%



SAGGI MICROBIOLOGICI: II DATASET

NOME COMPOSTO

KLEBSIELLA
PNEUMONIAE
sensibile ai
carbapenemi
MIC

Linalolo

$\leq 0,03\%$

Limonene

0,6%

Eucaliptolo

5%

alfa-pinene

>5%

Carvacrolo

$\leq 0,03\%$

Timolo

$\leq 0,03\%$

p-cimene

>5%

alfa-fellandrene

2,5%

4-carvomentenolo

$\leq 0,03\%$

gamma-terpinene

5%

Mircene

>5%

beta-pinene

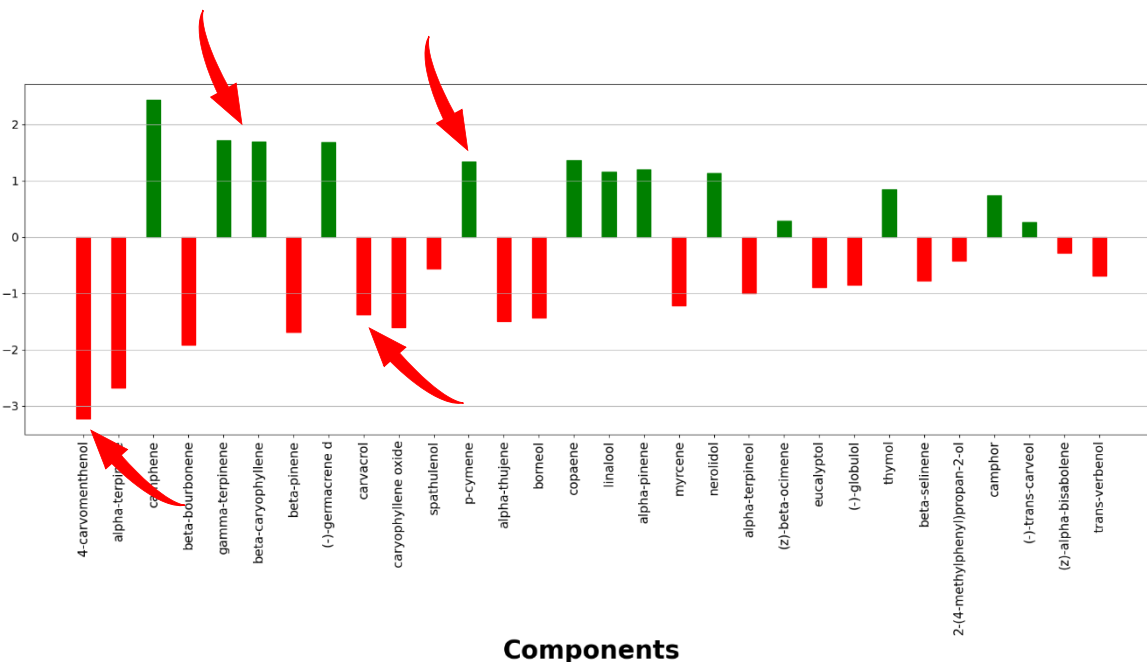
>5%

Terpinolene

5%

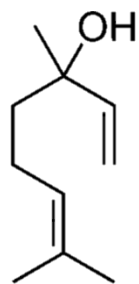
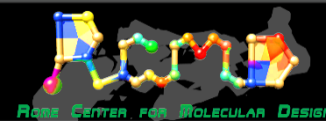
beta-cariofillene

>5%

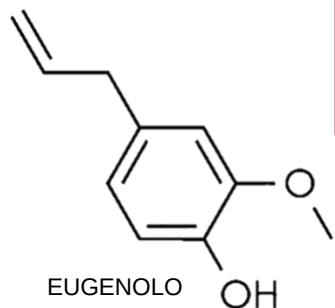




CONCLUSIONI



LINALOLO



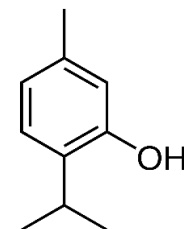
EUGENOLO

I DATASET

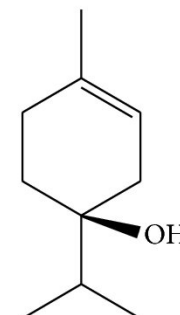
- ❖ **CARVACROLO**
- ❖ **TIMOLO**
- ❖ EUGENOLO
- ❖ CITRALE
- ❖ GERANIOLO

II DATASET

- ❖ LIMONENE
- ❖ LINALOLO
- ❖ **CARVACROLO**
- ❖ **TIMOLO**
- ❖ 4-CARVOMENTENOLO



TIMOLO



4-CARVOMENTENOLO

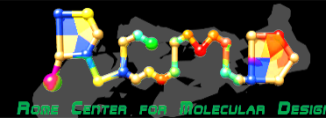


- **AGGIORNAMENTO DI MODELLI CON ACQUISIZIONE DI NUOVI DATI.**
- **TOSSICITA' COMPOSTI ALLE CONCENTRAZIONI STUDIE.**
- **PROGETTAZIONE DI OLI ESSENZIALI MEDIANTE MODELLI.**





RINGRAZIAMENTI



- ❖ Prof. Rino Ragno, relatore di tesi.
- ❖ Prof.ssa Alessandra Oliva, correlatrice di tesi.
- ❖ Il team RCMD: dott.ssa Roberta Astolfi, Dott. Filippo Sapienza e dott.ssa Eleonora Proia.
- ❖ Il team di Microbiologia: dott.ssa Maria Claudia Miele, dott.ssa Elisa D'Aliesio.



GRAZIE PER L'ATTENZIONE