

Sviluppo, validazione e interpretazione di modelli di classificazione ottenuti con algoritmi machine learning applicati a dati di composizione e attività antimicrobica (*E. Coli*) di oli essenziali.



SAPIENZA
UNIVERSITÀ DI ROMA

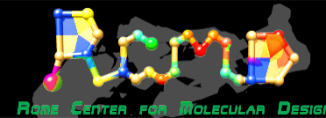
Facoltà di Farmacia e Medicina
Corso di laurea in Chimica e tecnologia farmaceutiche
Tesi sperimentale in Chimica Farmaceutica
A.A. 2022/2023

Laureanda: Giulia Dell'Aquila
Matricola: 1644916

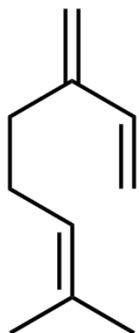
Relatore: Prof. Rino Ragno



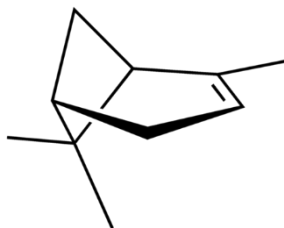
Oli essenziali



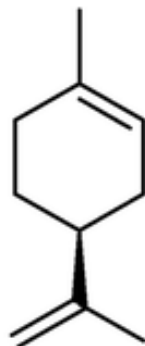
Composti monoterprenici



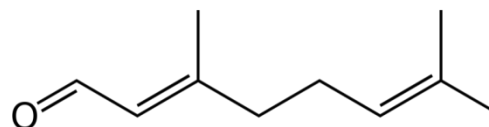
Mircene



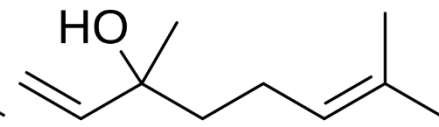
α -Pinene



D-Limonene

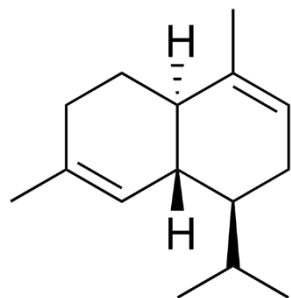


Geraniale

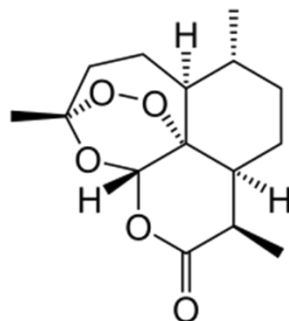


Linanolo

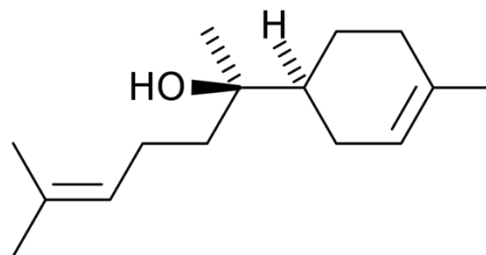
Composti sesquiterpenici



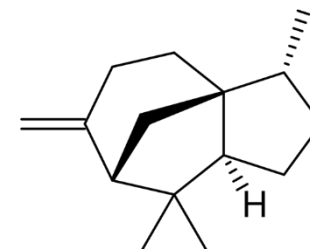
α -Cadinene



Artemisinina



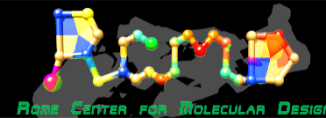
α -Bisabololo



β -Cedrene



Oli essenziali



- **Antibatterica**
“High Potency of Melaleuca alternifolia Essential Oil against Multi-Drug Resistant Gram-Negative Bacteria and Methicillin-Resistant Staphylococcus aureus”
Oliva A., Costantini S., De Angelis M., Garzoli S., Božović M., Mascellino M.T., Vullo V., Ragno R.
Molecules, 2018.
- **Antimicotica**
“Effects of Mentha suaveolens Essential Oil Alone or in Combination with Other Drugs in Candida albicans”
Stringaro A., Vavala E., Colone M., Pepi F., Mignogna G., Garzoli S., Cecchetti S., Ragno R., Angiolella L.
Evidence-Based Complementary and Alternative Medicine, 2014.
- **Antivirale**
“In vitro inhibition of herpes simplex virus type 1 replication by Mentha suaveolens essential oil and its main component piperitenone oxide”
Civitelli L., Panella S., Marcocci M.E., De Petris A., Garzoli S., Pepi F., Vavala E., Ragno R., Nencioni L., Palamara A.T., Angiolella L.
Phytomedicine, 2014.
- **Antiossidante**
“Oxidative DNA damage preventive activity of essential oils of three Pinus species: P. mugo, P. sibirica, and P. silvestre”
Matić S.Lj., Mladenović T.M., Mladenović M.P., Tomašević N.M., Capobianco R., Ragno A., Sapienza F.U., Astolfi R., Ragno R.
ICCBKIG, 2023.
- **Antinfiammatoria**
“Calamintha nepeta (L.) Savi and its Main Essential Oil Constituent Pulegone: Biological Activities and Chemistry”
Božović M., Ragno R.
Molecules, 2017.
- **Antitumorale**
“Pinus mugo Essential Oil Impairs STAT3 Activation through Oxidative Stress and Induces Apoptosis in Prostate Cancer Cells”
Thalappil M.A., Butturini E., Carcereri de Prati A., Bettin I., Antonini L., Sapienza F.U., Garzoli S., Ragno R., Mariotto S.
Molecules, 2022.



AI4EssOil

HOME THE PROJECT SEARCH PREDICT CITE US LOGIN

Welcome AI4EssOil

ROME CENTER FOR MOLECULAR DESIGN

Explore thousand of essential oils based on
hundreds of publications

2756

Extracts
compositions

1107

Plants

1243

Publications
analysed

20950

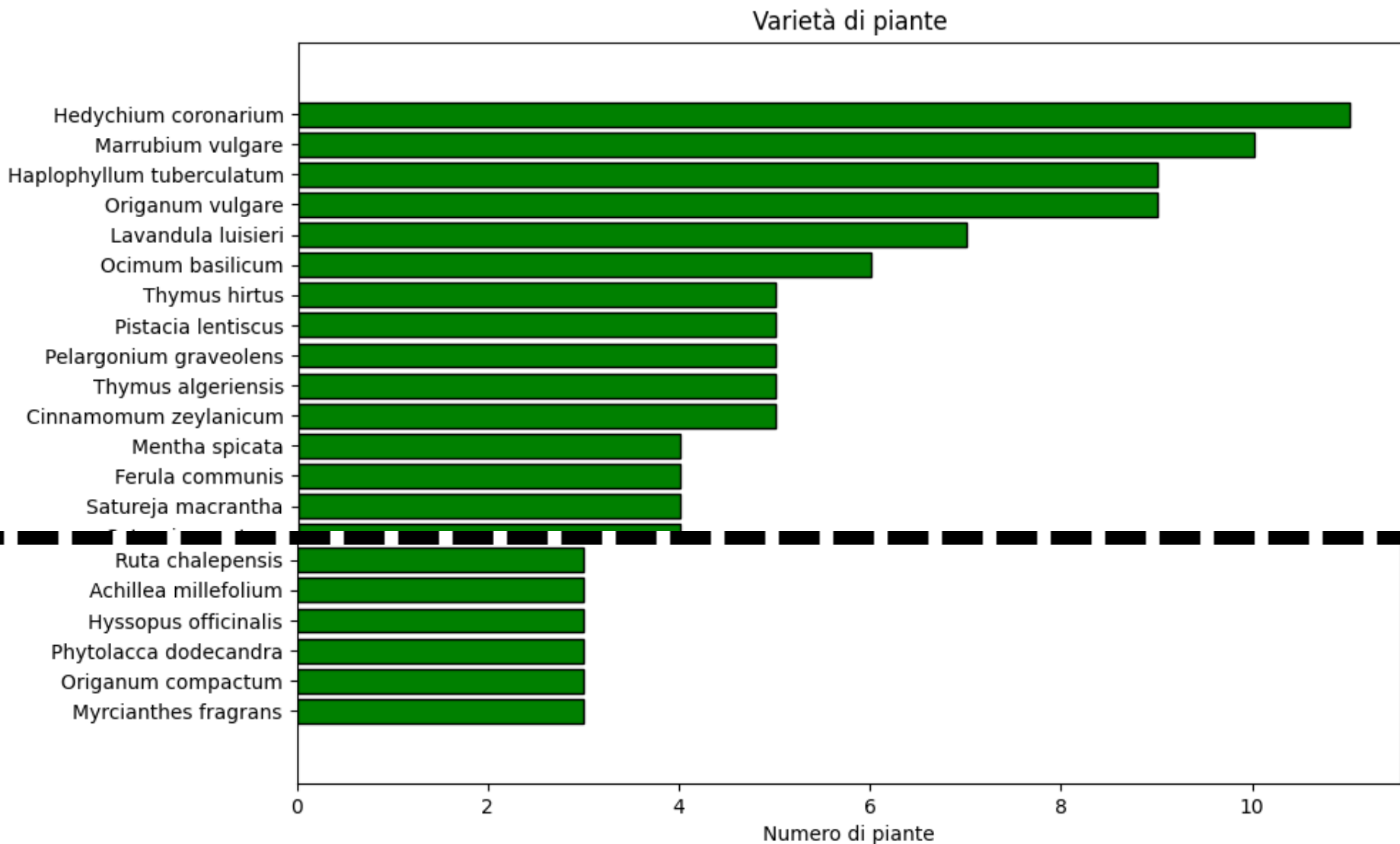
Biological activities
stored



Organism	Target	Target Code	Activity Value	Activity Unit	Activity Std Value	Activity Std Unit	Incubation Time	Activity Type	Fixed Doses Value	Activity Mode
Bacteria G-	Escherichia Coli	PTCC 1338	150.0	ug/ml	1.500e-02	% pv	24 h	MIC	None	Microdilution
Bacteria G-	Escherichia Coli	ATCC 25922	6.25	mg/ml	6.250e-01	% pv	24 h	MIC	None	Microdilution
Bacteria G-	Escherichia Coli	ATCC 25922	12.5	mg/ml	1.250e+00	% pv	24 h	MIC	None	Microdilution
Bacteria G-	Escherichia Coli	ATCC 10536	500.0	ug/ml	5.000e-02	% pv	24 h	MIC	None	Microdilution
Bacteria G-	Escherichia Coli	None	0.8	%	8.000e-01	%		MIC	None	Microdilution
Bacteria G-	Escherichia Coli	ATCC 8739	0.8	%	8.000e-01	%		MIC	None	Microdilution
Bacteria G-	Escherichia Coli	ATCC35210	0.03	mg/ml	3.000e-03	% pv	24 h	MIC	None	Microdilution
Bacteria G-	Escherichia Coli	ATCC35210	0.03	mg/ml	3.000e-03	% pv	24 h	MIC	None	Microdilution
Bacteria G-	Escherichia Coli	P1420	6.25	mg/l	6.250e+00	mg/l	24 h	MIC	None	Microdilution
Bacteria G-	Escherichia Coli	P1420	6.25	mg/l	6.250e+00	mg/l	24 h	MIC	None	Microdilution

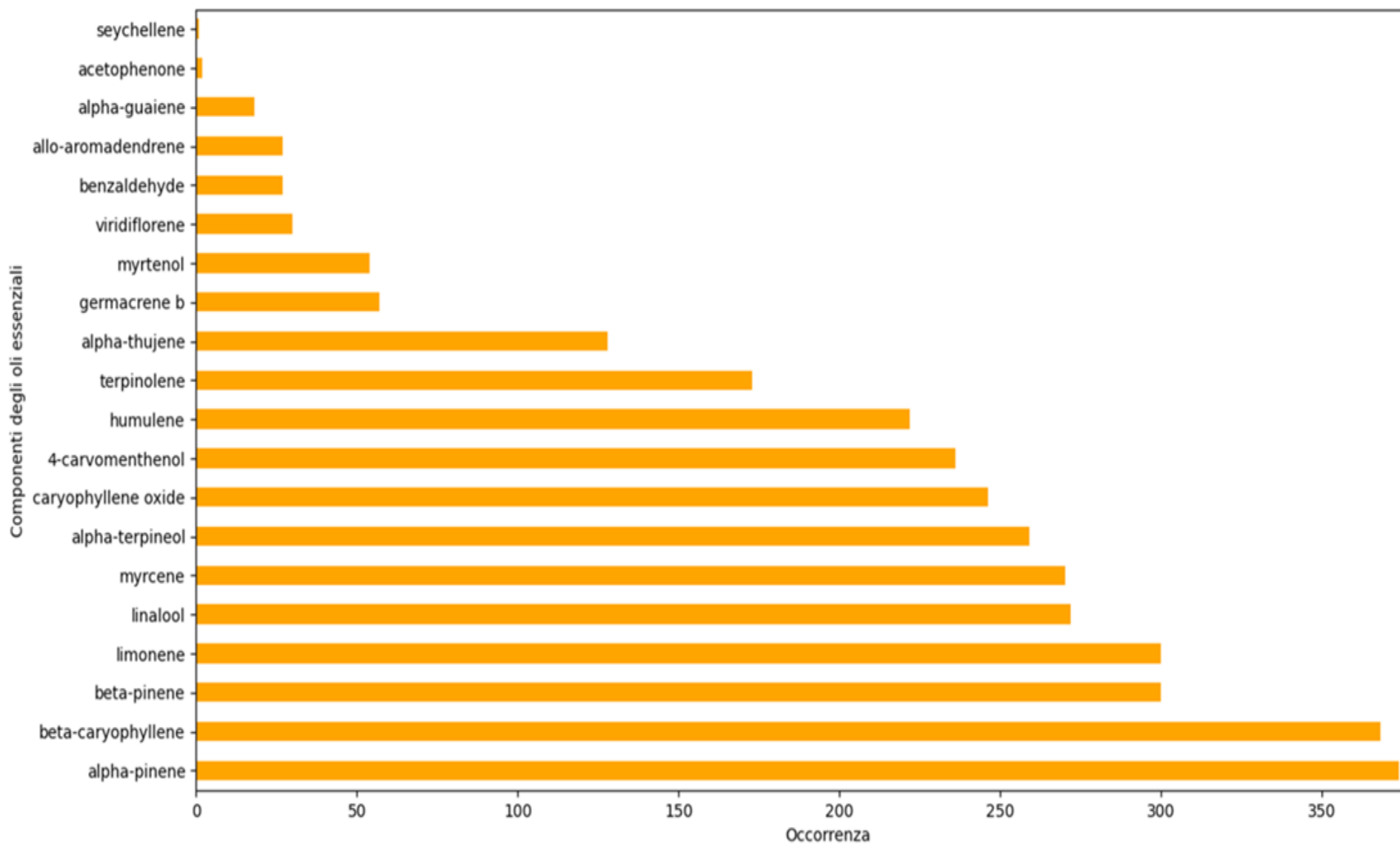
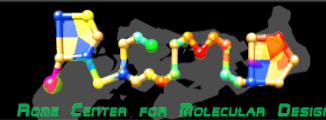


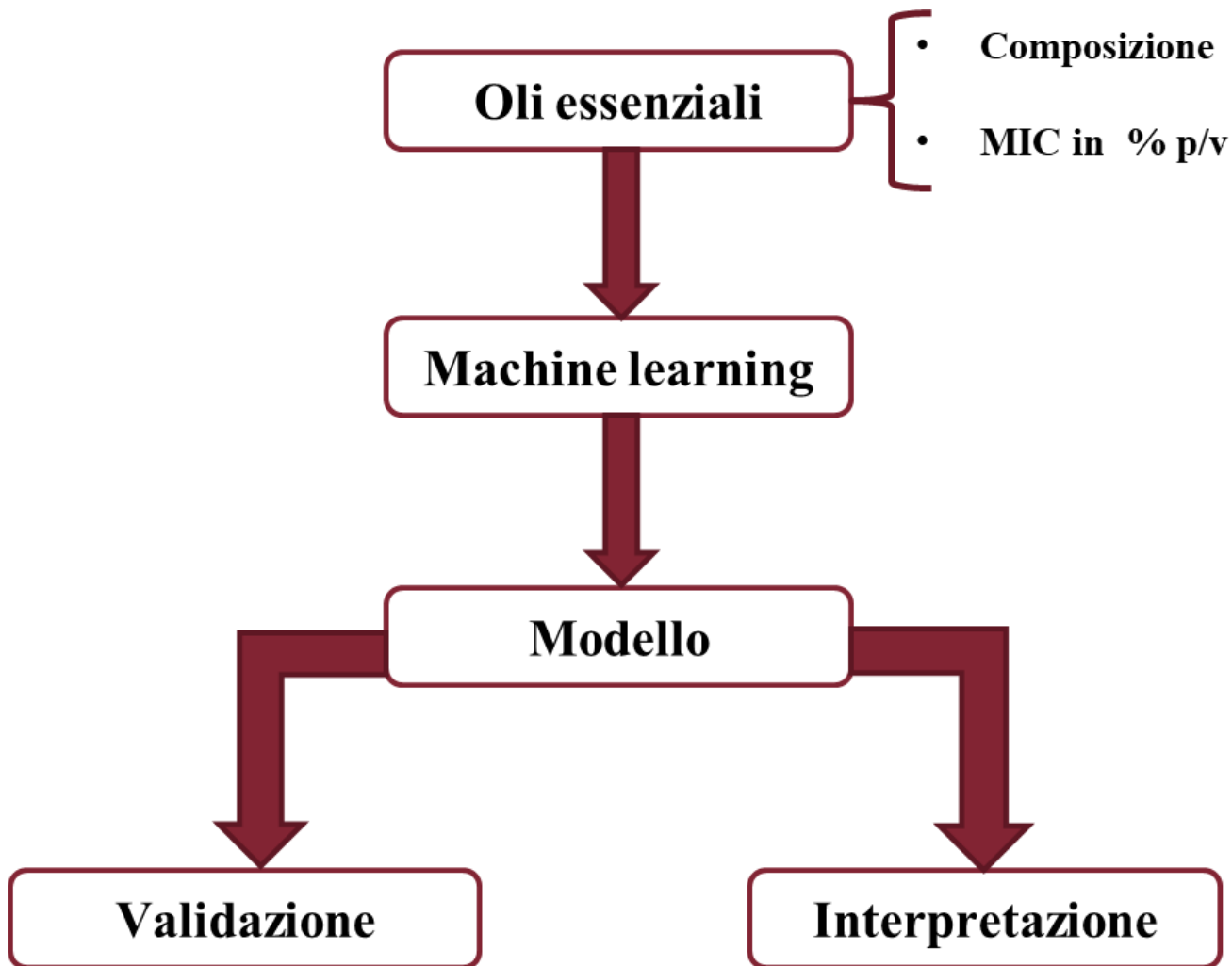
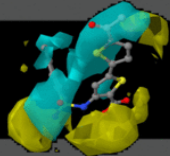
Oli essenziali utilizzati





Oli essenziali utilizzati







python

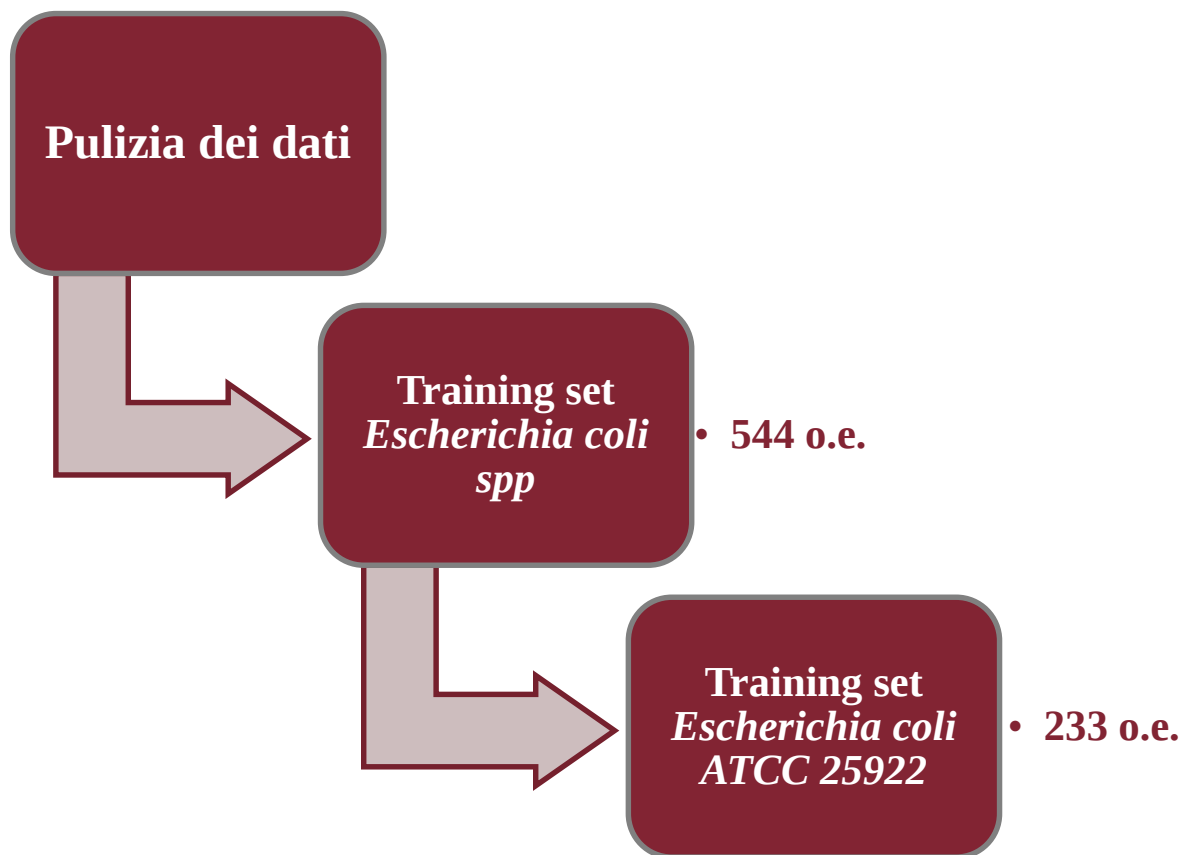


jupyter notebook

Welcome to jupyter.rcmd.it

We have increased the number of servers, here you have a list of them. Thesis students are only allowed to use i7 machines. Please log the most free one (the one with highest CPU IDLE percentage).

jupyter-i71.rcmd.it	jupyter-i72.rcmd.it	jupyter-i73.rcmd.it	jupyter-i74.rcmd.it	jupyter-i75.rcmd.it
jupyter-cl101.rcmd.it	jupyter-cl102.rcmd.it	jupyter-cl103.rcmd.it	jupyter-cl104.rcmd.it	jupyter-cl105.rcmd.it
jupyter-cl106.rcmd.it	jupyter-cpu1.rcmd.it	jupyter-cpu2.rcmd.it	jupyter-gpu1.rcmd.it	jupyter-gpu2.rcmd.it
jupyter-gpu3.rcmd.it	jupyter-gpu4.rcmd.it	jupyter-gpu5.rcmd.it		





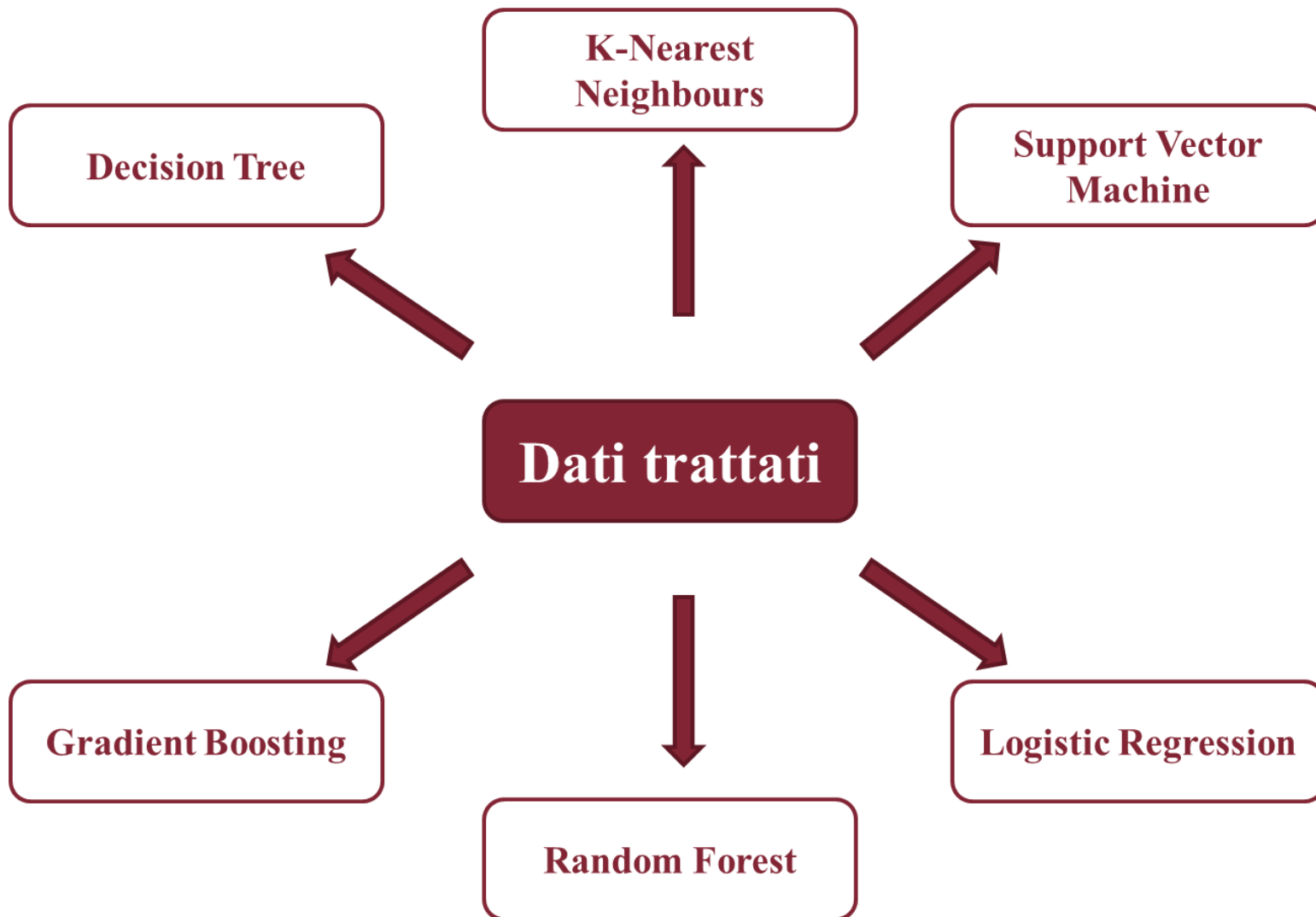
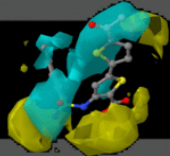
Escherichia coli spp

Escherichia coli
ATCC 25922



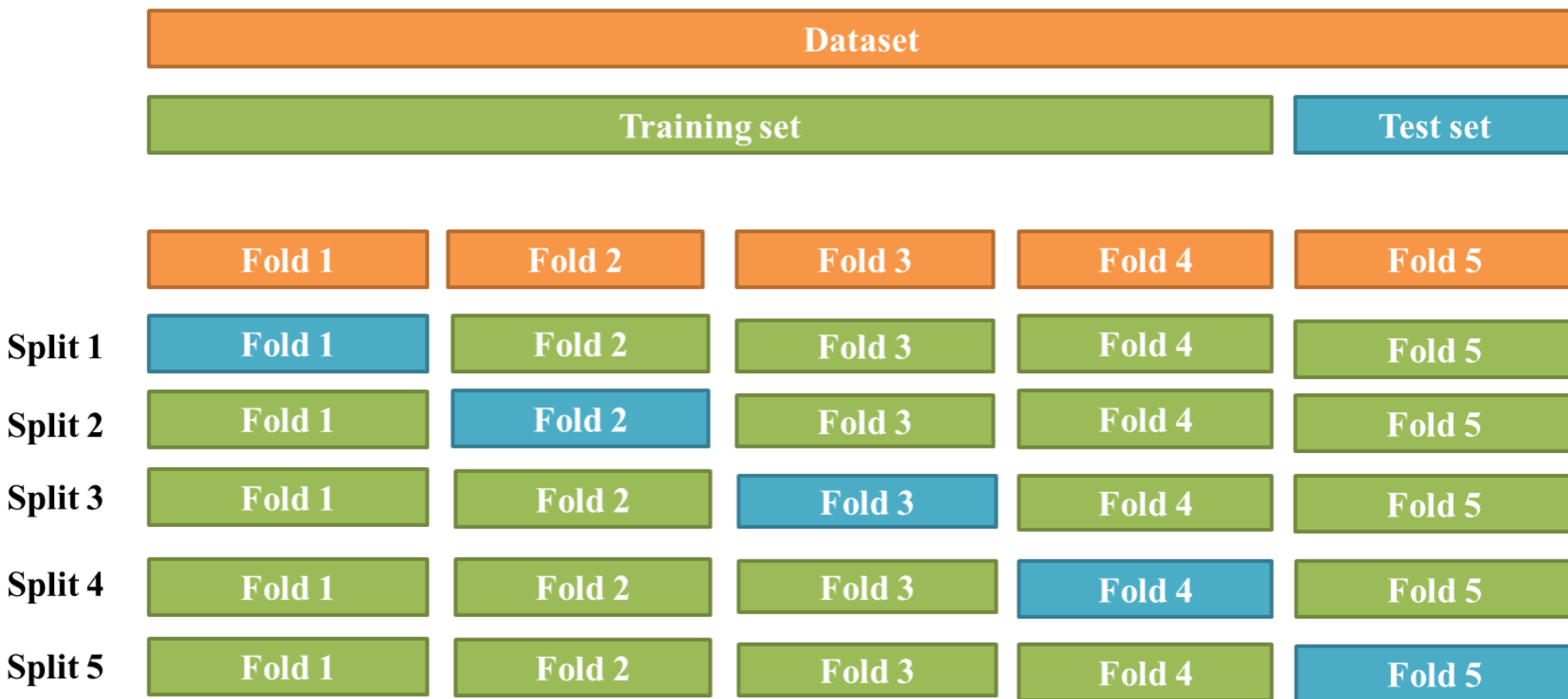
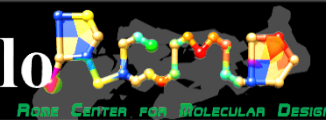
Pretreatment

- MinMaxScaler
- Nlevels
- PCA





Valutazione della robustezza del modello



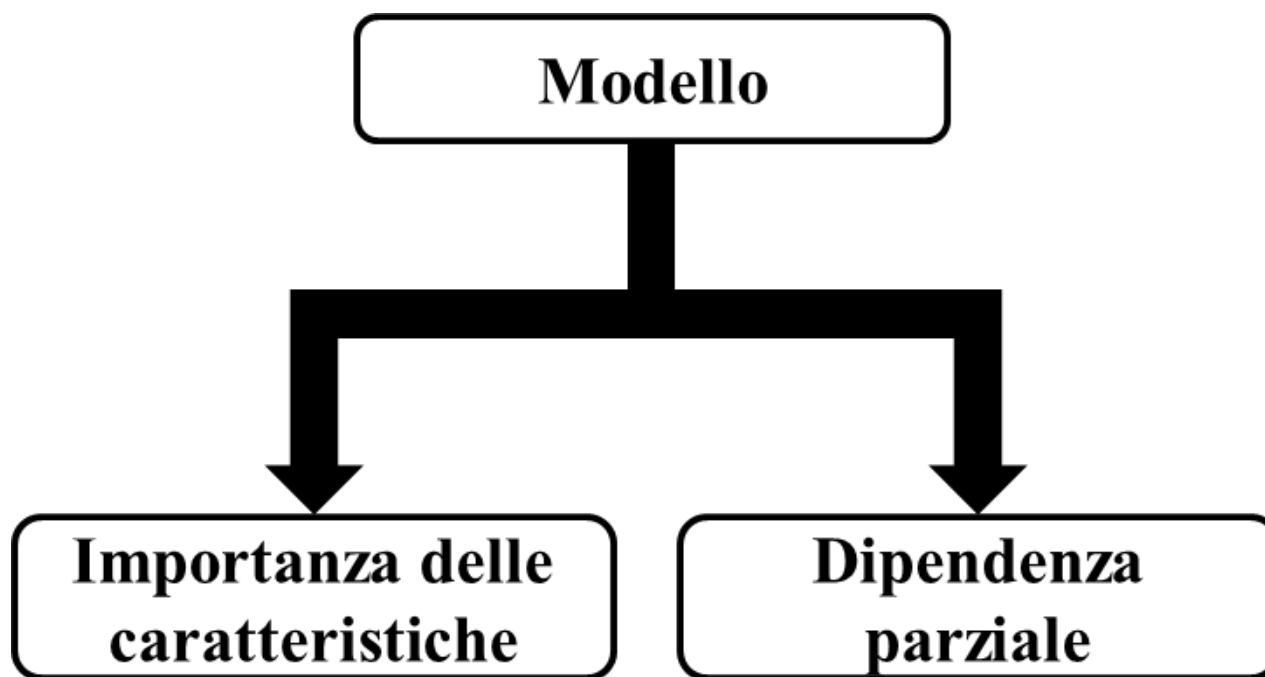


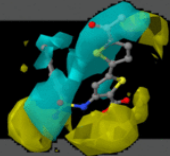
- **Coefficiente di Correlazione di Matthews:**

$$MCC = \frac{(TP \times TN) - (FP \times FN)}{\sqrt{(TP+FP) \times (TP+FN) \times (TN+FP) \times (TN+FN)}}$$

- **Coefficiente di Correlazione di Matthews Normalizzato:**

$$NMCC = \frac{MCC + 1}{2}$$



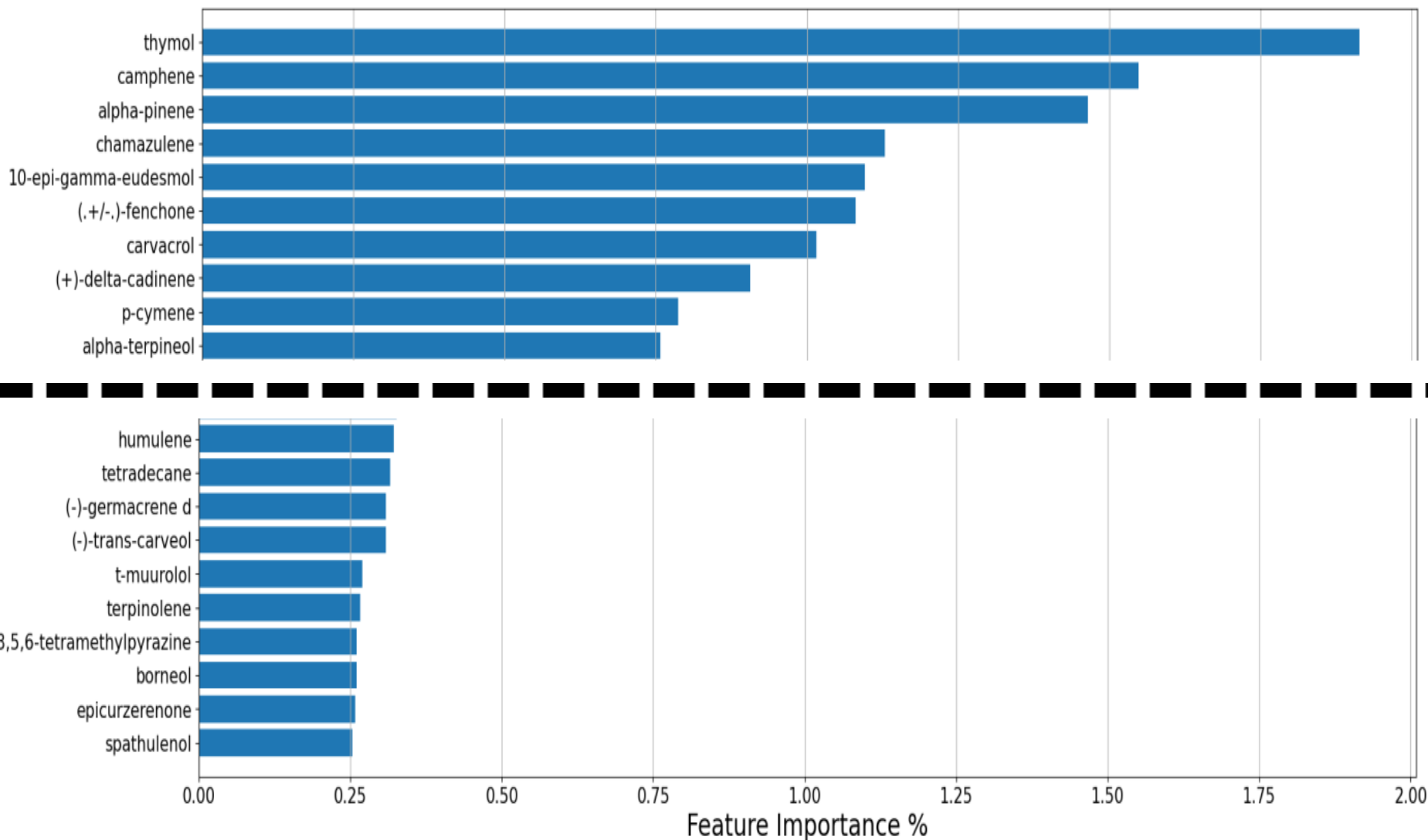
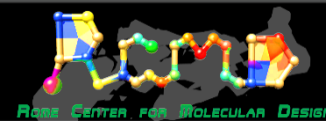


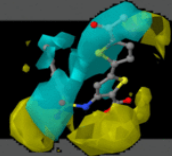
SUPPORT VECTOR MACHINE

threshold	0.01 % p/v
nlevel	0
scaling	1
pca	0
norm_mcc_pred_average	0.61
norm_mcc_fit	0.92
norm_mcc_cv	0.61

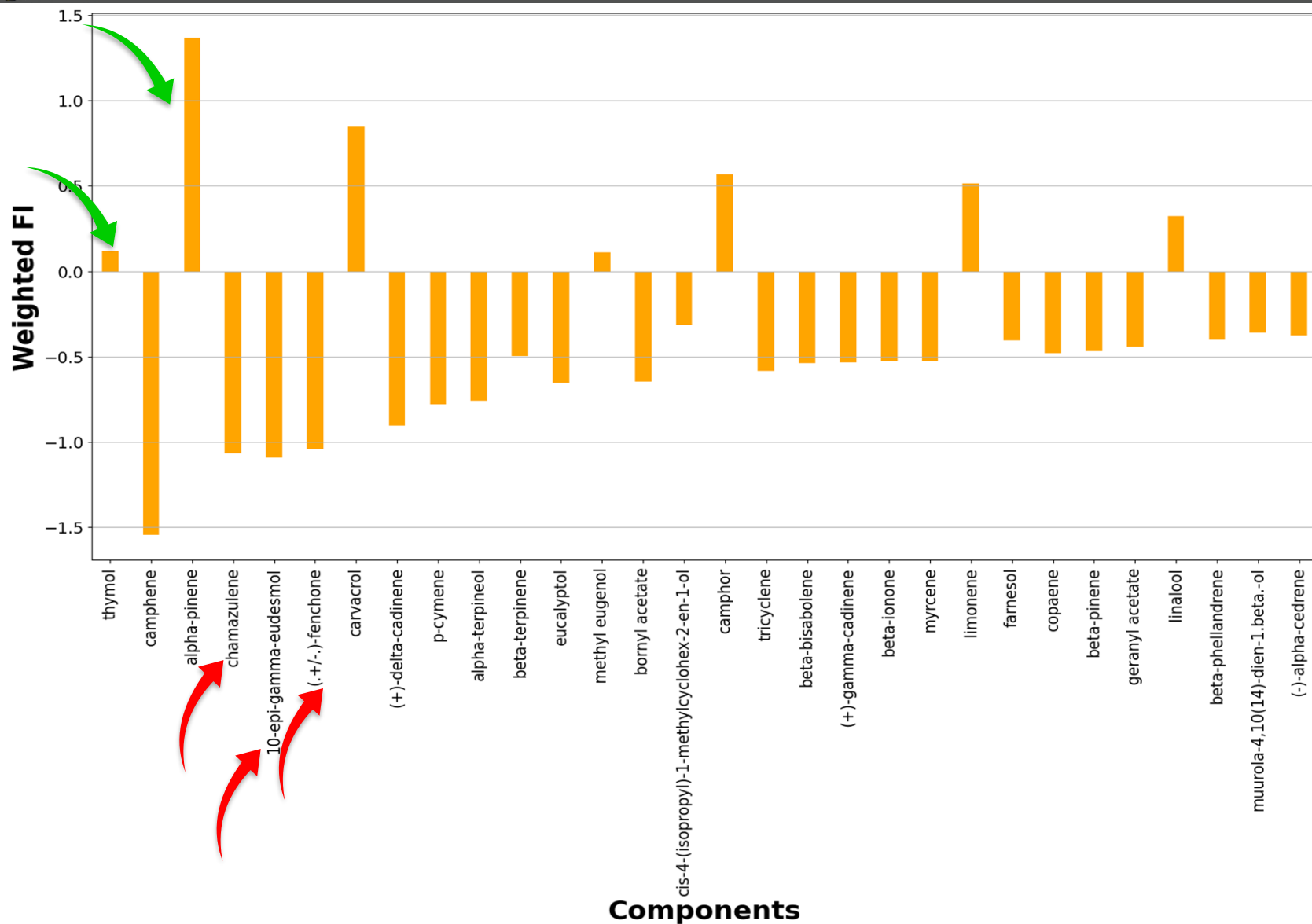


Importanza dei componenti – *Escherichia coli* spp

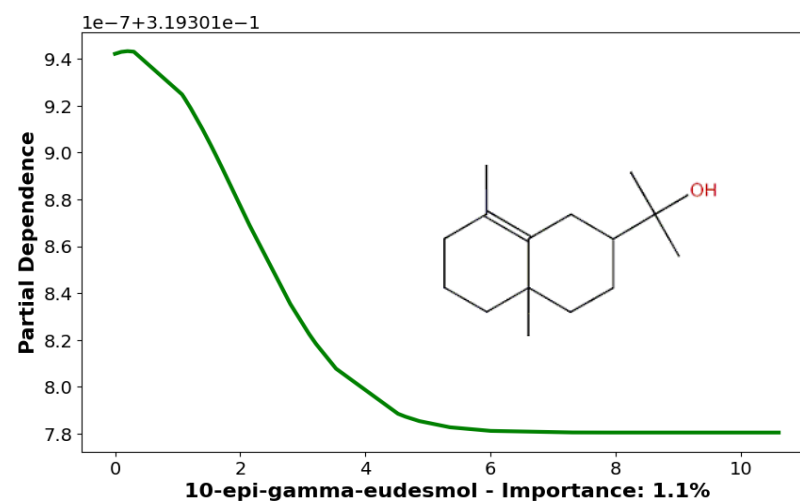
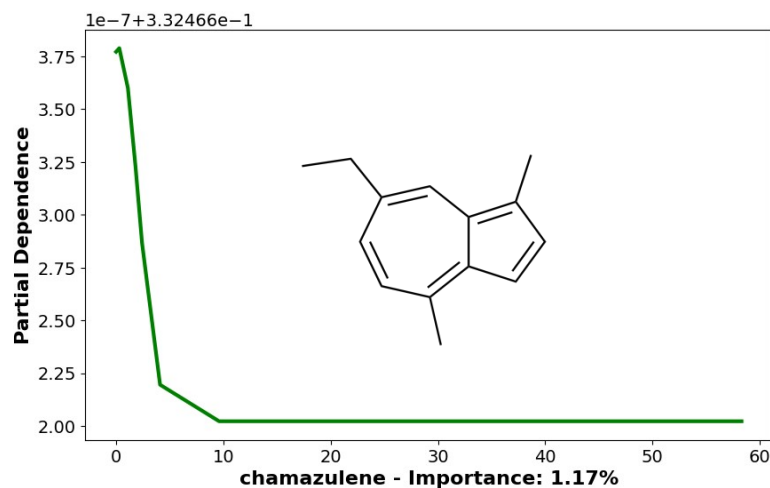
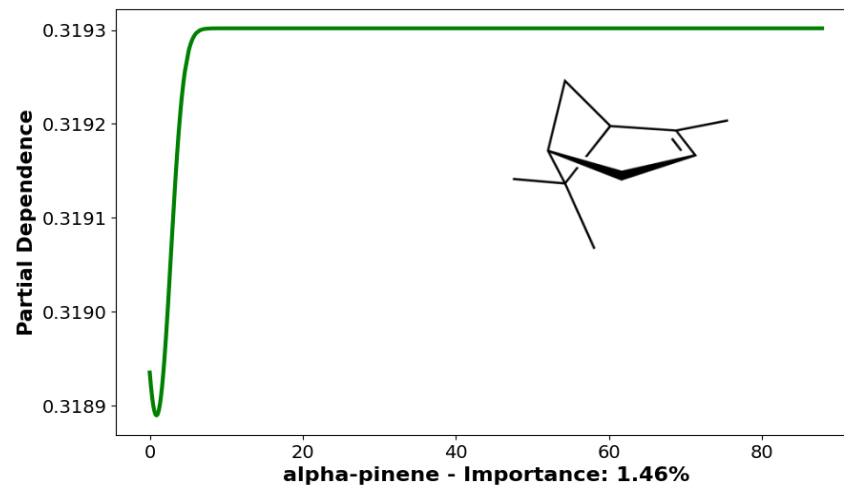
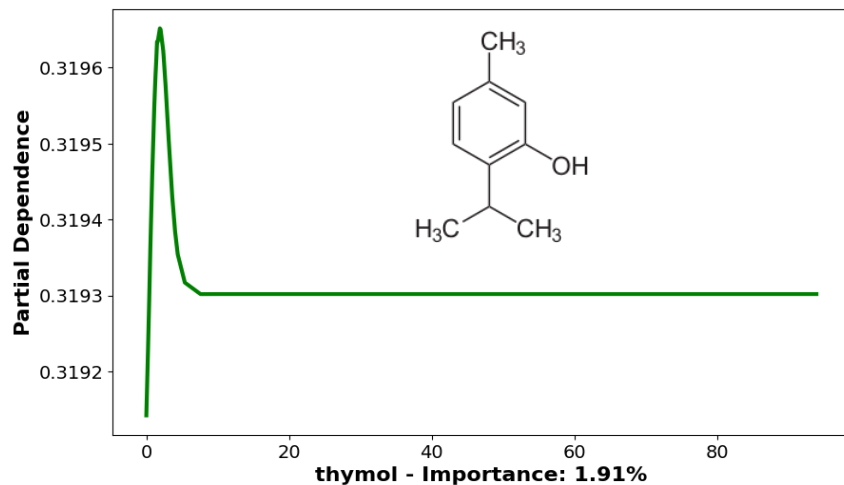


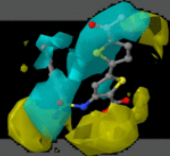


Dipendenza parziale – *Escherichia coli* spp



Dipendenza parziale – *Escherichia coli* spp



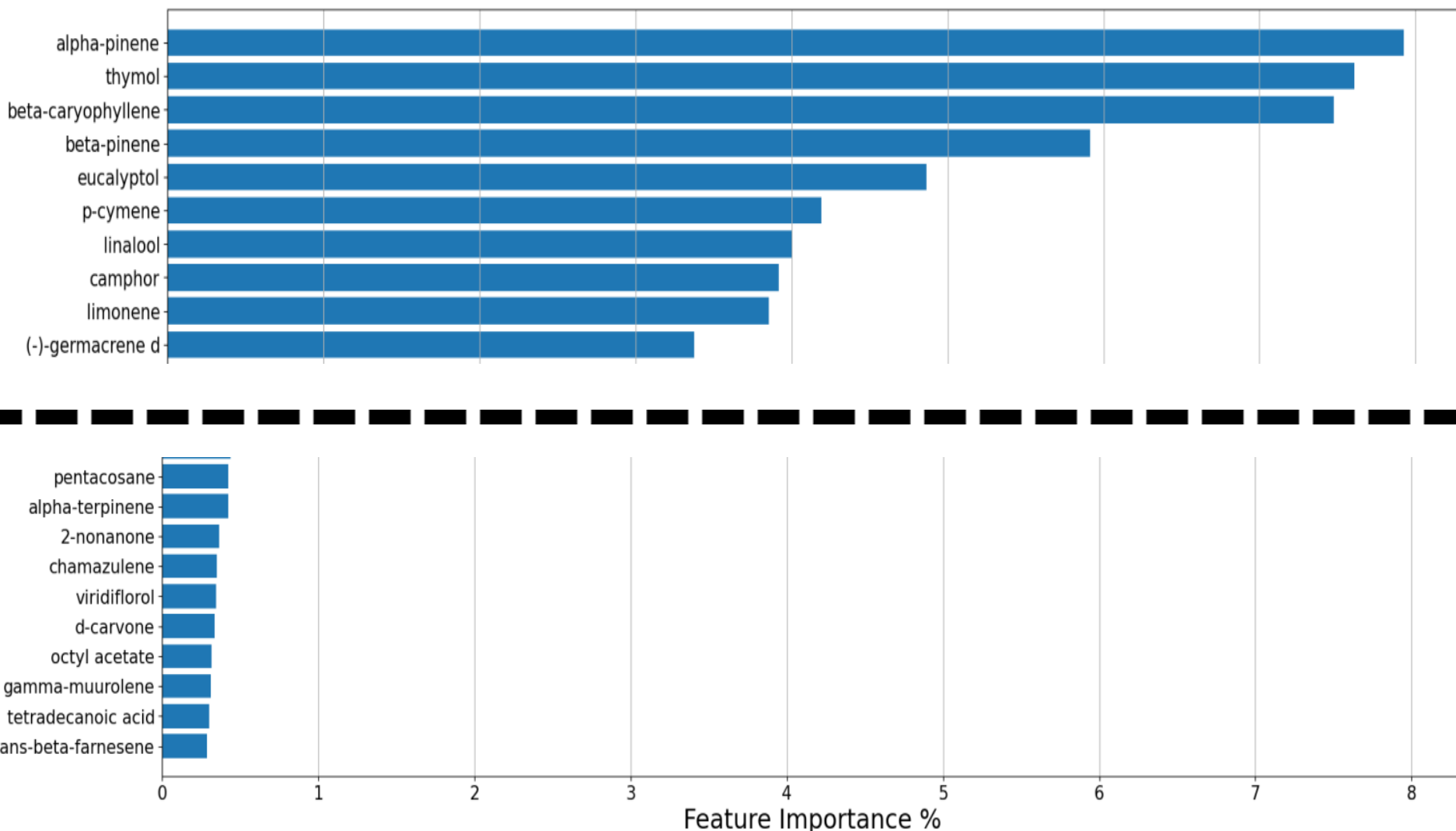
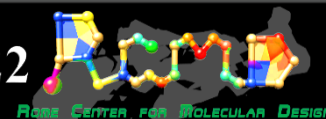


GRADIENT BOOSTING

threshold	0.009 % p/v
nlevel	2
scaling	0
pca	0.7
norm_mcc_pred_average	0.69
norm_mcc_fit	0.65
norm_mcc_cv	0.55

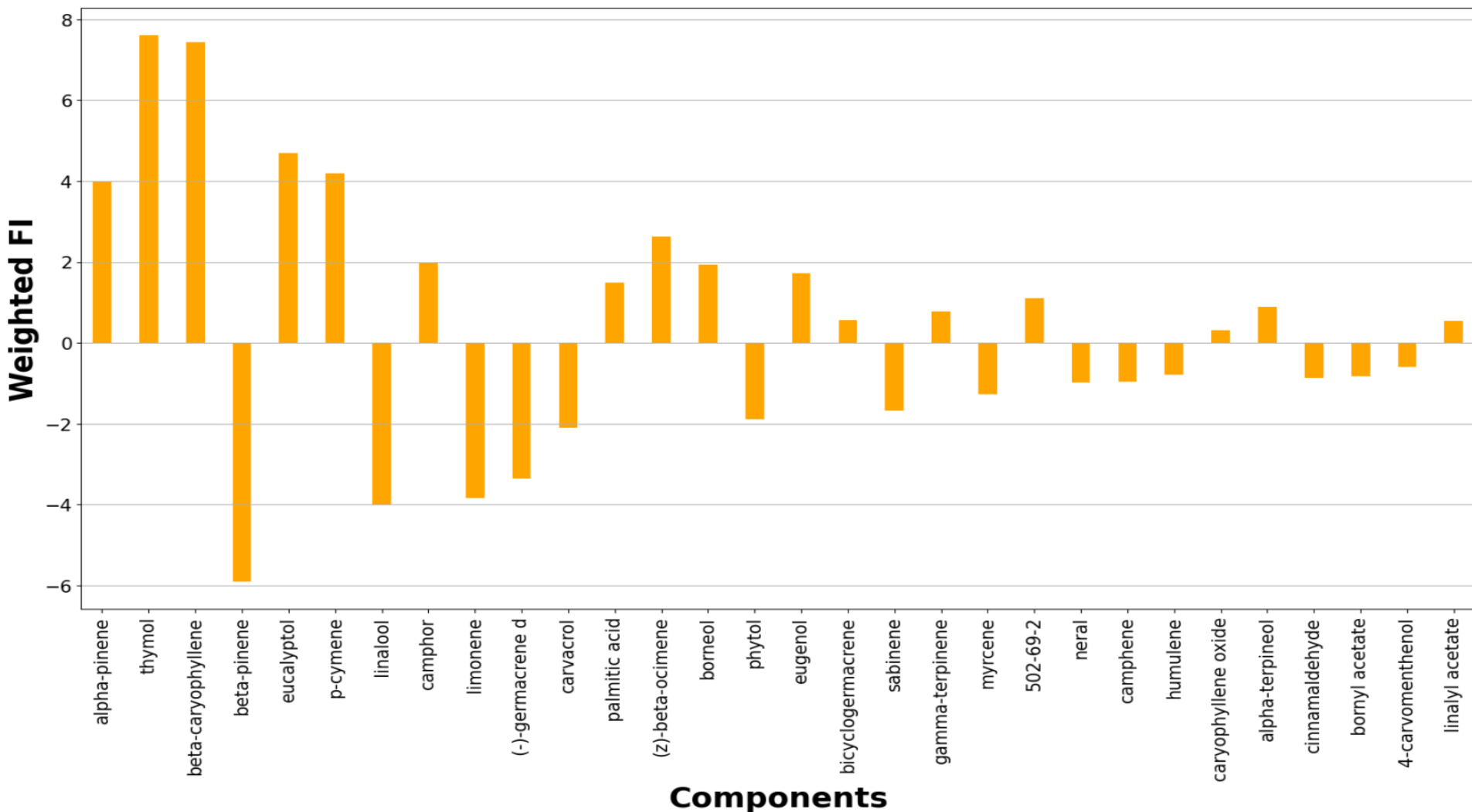
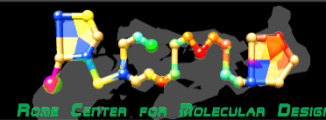


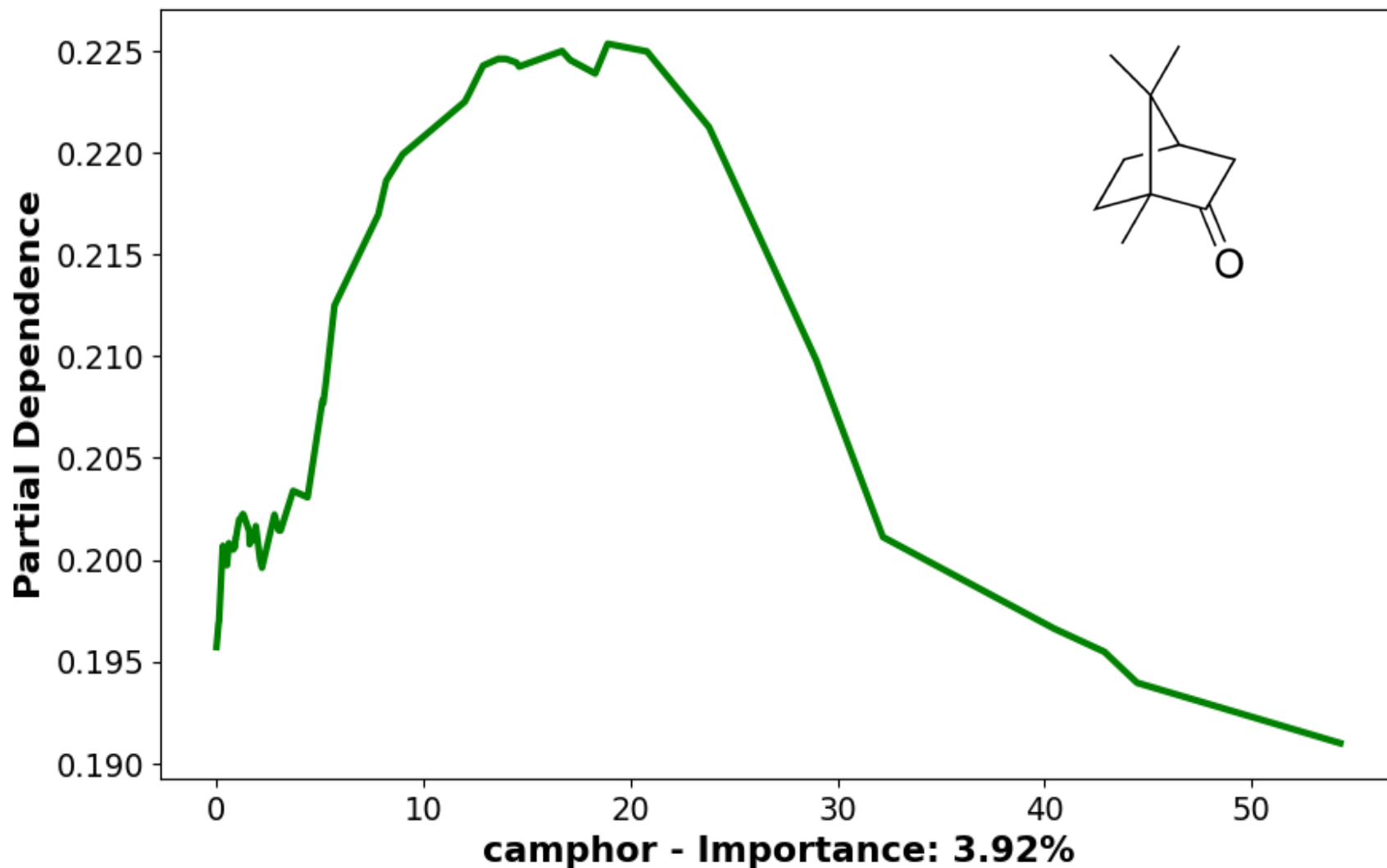
Importanza dei componenti – *Escherichia coli* ATCC 25922





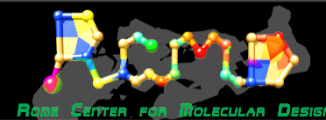
Dipendenza parziale – *Escherichia coli* ATCC 25922







Validazione esterna



Validation set



Modello
E. coli spp



Totale predizioni
corrette
100 %

Validation set



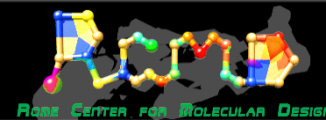
Modello
E. Coli ATCC 25922



Totale predizioni
corrette
95,1 %



Conclusioni



- **Attività globale** ✓
- **Dipendenza parziale delle componenti** ✓



Prospettive future



- **Componenti con influenza positiva ...**

- **Componenti con influenza negativa...**

“Antimicrobial and Antibiofilm Activity and Machine Learning Classification Analysis of Essential Oils from Different Mediterranean Plants against Pseudomonas aeruginosa”

Artini M., Patsilinakos A., Papa R., Božović M., Sabatino M., Garzoli S., Vrenna G., Tilotta M., Pepi F., Ragno R., Selan L.

Molecules, 2018.

“Essential Oils Biofilm Modulation Activity, Chemical and Machine Learning Analysis—Application on Staphylococcus aureus Isolates from Cystic Fibrosis Patients”

Papa R., Garzoli S., Vrenna G., Sabatino M., Sapienza F.U., Relucenti M., Donfrancesco O., Fiscarelli E.V., Artini M., Selan L., Ragno R.

International Journal of Molecular Sciences, 2020.

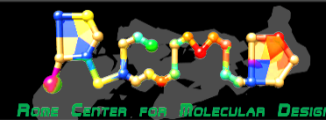
“Multistate Outbreak of Melioidosis Associated with Imported Aromatherapy Spray”

Jay E. Gee, Ph.D., William A. Bower, M.D., Amber Kunkel, Sc.D.

The new England Journal of Medicine, 2022.



Ringraziamenti



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E tutti dottori e studenti del lab RCMD



Grazie per l'attenzione!

