"SHELF-LIFE PREDICTIVE MODEL STUDY OF BOTTLED EXTRA VIRGIN OLIVE OIL BASED ON THE ANALYSIS OF HEAD SPACE AROMATIC MOLECULES"

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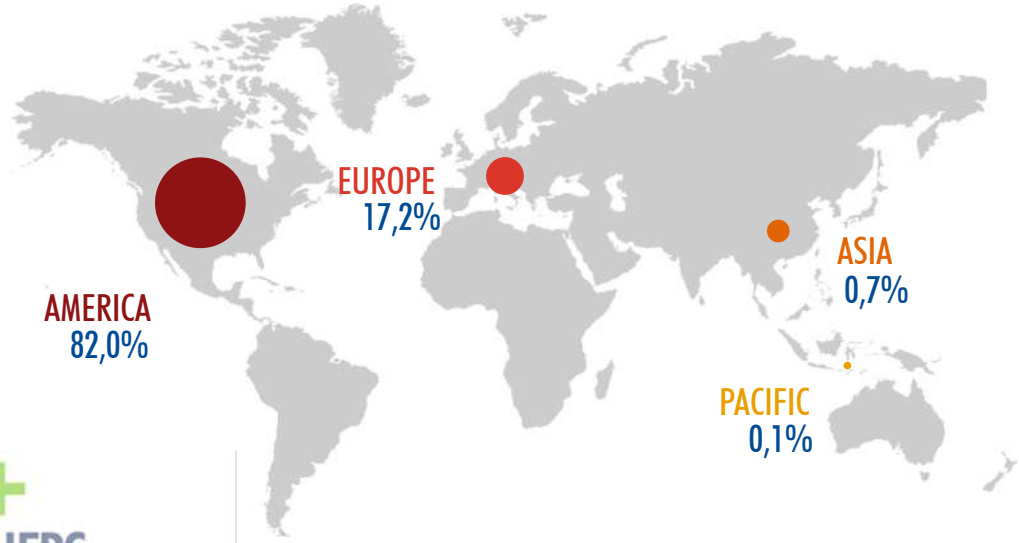
"EDIBLE OILS AND FATS: INNOVATION AND SUSTAINABILITY IN PRODUCTION AND CONTROL"
PERUGIA (IT), JUNE 15th -17th, 2022

MEET AGRITALIA

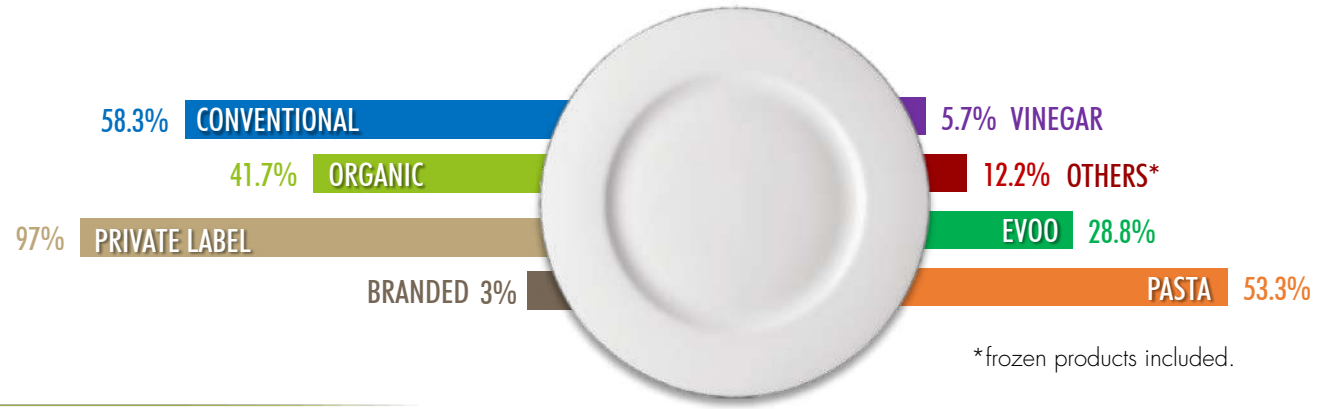
- R&D of innovative items
- Supervision of the raw materials markets and production processes
- Suppliers' qualification by internal audits
- Integrated logistics services
- Marketing support, art-work & printing assistance
- Quality Assurance testing program
- Financial services and currency fixing



3,000+ CONTAINERS SHIPPED TO U.S. IN 2021

700+ PRODUCTS OFFERED

100+ CERTIFIED SUPPLIERS



*frozen products included.

AGRITALIA SENSORY CHEMICAL SYSTEM

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To protect its customers and monitor the supplying process, Agritalia has designed, implemented and eventually certified an innovative system for the approval of olive oil batches called ASCS (Agritalia Sensory Chemical System).

This system involves chemical and sensory evaluations of the batch before bottling following a detailed procedure.

Even after bottling, the oil is monitored through:

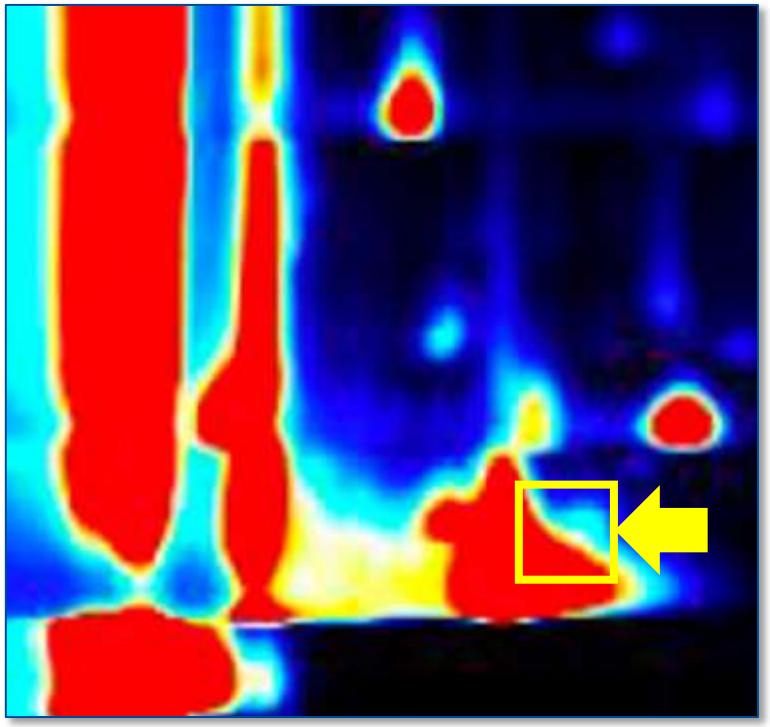
a. sampling from shelf at customers' stores with subsequent analysis
b. end of shelf-life analysis as required by customers' analysis plan

As part of this strategic activity, Agritalia started a researched aimed at studying the shelf-life of EVOOs based on volatiles and a 20-month timeframe.

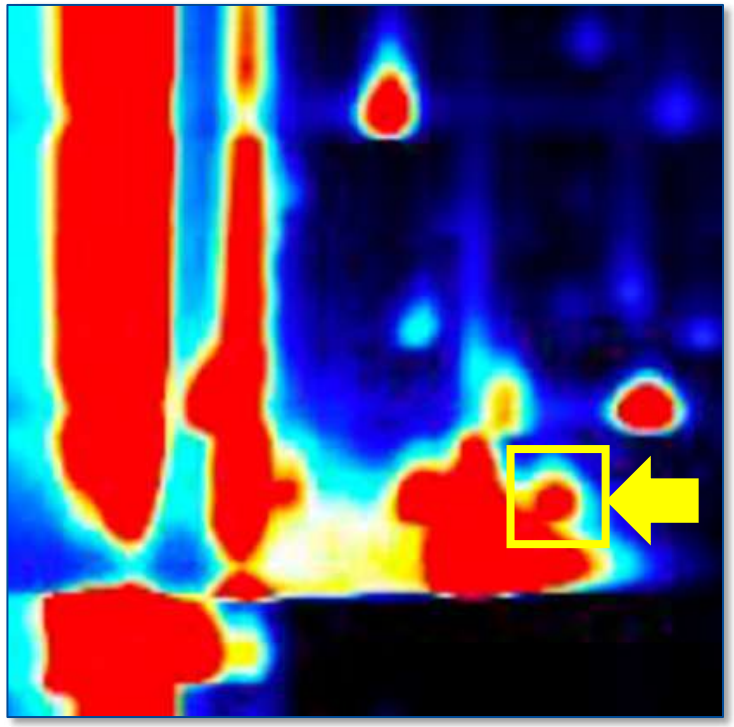
WHEN IT ALL BEGAN

The idea of using the head-space odorous molecules to predict the age of bottled extra virgin olive oil was born some years ago from the observations on a specific sample of extra virgin olive oil judged rancid by the official control panels.

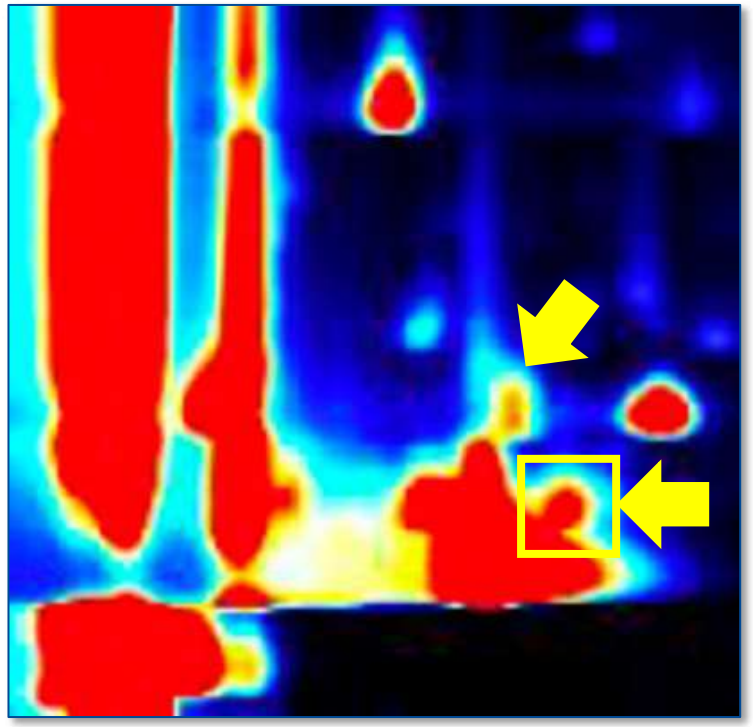
EVOO: NO DEFECTS



SLIGHTLY RANCID



RANCID



The development of strange odorous molecules during the store of oil bottles on shelf.

R&D OBJECTIVES

a. Explore the possibility of deriving a shelf-life empirical model through the study of head-space odorous molecules;

b. Elaborate the model on the basis of the extra virgin olive oils marketed by Agritalia: Mediterranean blend (conventional and organic), olive oil blends of Italian, Spanish and Greek origin;

c. Apply a purely industrial, empirical approach, based on the most advanced methodology available.

$$Months_{sample\text{-}i} = f(VOC_i)$$

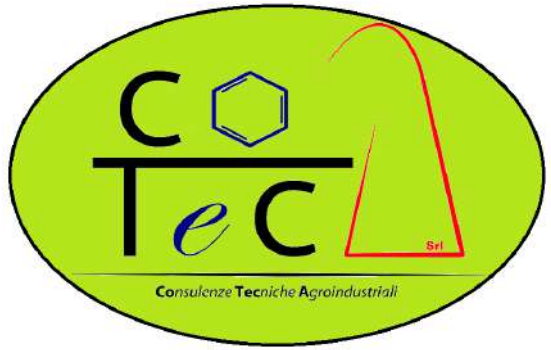
- UNTARGETED DATA
- HS-SPME-GC/MS
- MACHINE LEARNING, HEMOMETRICS

DATA SAMPLING

Bottled extra virgin olive oil samples	#
Mediterranean blend	4
Organic Mediterranean blend	3
Italian	1
Spanish	2
Greek	2
Validation sample from MFS (monitoring from shelf)	57

Picking times (month)	Y
0 months	0
4 months	4
8 months	8
12 months	12
16 months	16
20 months	20

Samples recap	#
Extra virgin olive oil bottles stored	72
Extra virgin olive oil bottles from MFS	57
HS-SPME-GC/MS CoA	129
Odorous molecules	71



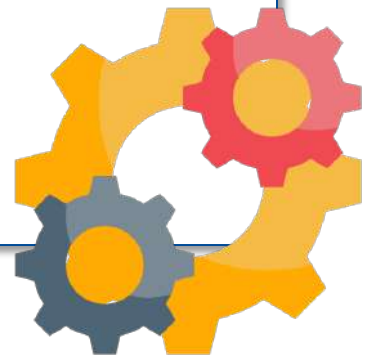
doi.org/10.1016/j.talanta.2016.12.082

Acetic acid, methyl ester	Butanoic acid	1-Octen-3-ol
1-Propanol	Octane	2-Octanone
2-Butanone	Hexanal	2-Octanol
Acetic acid	Butanoic acid, ethyl ester	Octanal
2-Butanol	Acetic acid, butyl ester	3-Hexen-1-ol, acetate
Ethyl Acetate	3-Hexenal	2,4-Heptadienal
1-Propanol, 2-methyl	2-Hexenal	Acetic acid, hexyl ester
Methyl propionate	3-Hexen-1-ol	2-Hexen-1-ol, acetate
Butanal, 3-methyl	3-Hexen-1-ol	D-Limonene
Butanal, 2-methyl	2-Hexen-1-ol	2-Octenal
1-Penten-3-ol	2-Hexen-1-ol	1-Octanol
1-Penten-3-one (EthylVinylKetone)	1-Hexanol	Phenol, 2-methoxy(Guaiacol)
Propanoic acid	Pentanoic acid	2-Nonanone
3-Pentanone	2-Heptanone	Nonanal
Pentanal	Heptanal	Phenylethyl Alcohol
Heptane	2-Heptanol	2-NonenalE
(R)-(-)-2-Pentanol	2,4-Hexadienal	Phenol 4-ethyl
Propanoic acid, ethyl ester	2-HeptenalE	1-Nonanol
1-Butanol, 3-methyl	Benzaldehyde	Decanal
1-Butanol, 2-methyl	1-Heptanol	2,4-Nonadienal
2-PentenalE	1-Octen-3-one	2-Decenal
1-Pentanol	Hexanoic acid	Phenol, 4-ethyl-2-methoxy
2-Penten-1-ol	Phenol	2,4-Decadienal
2-Penten-1-ol	5-Hepten-2-one, 6-methyl	

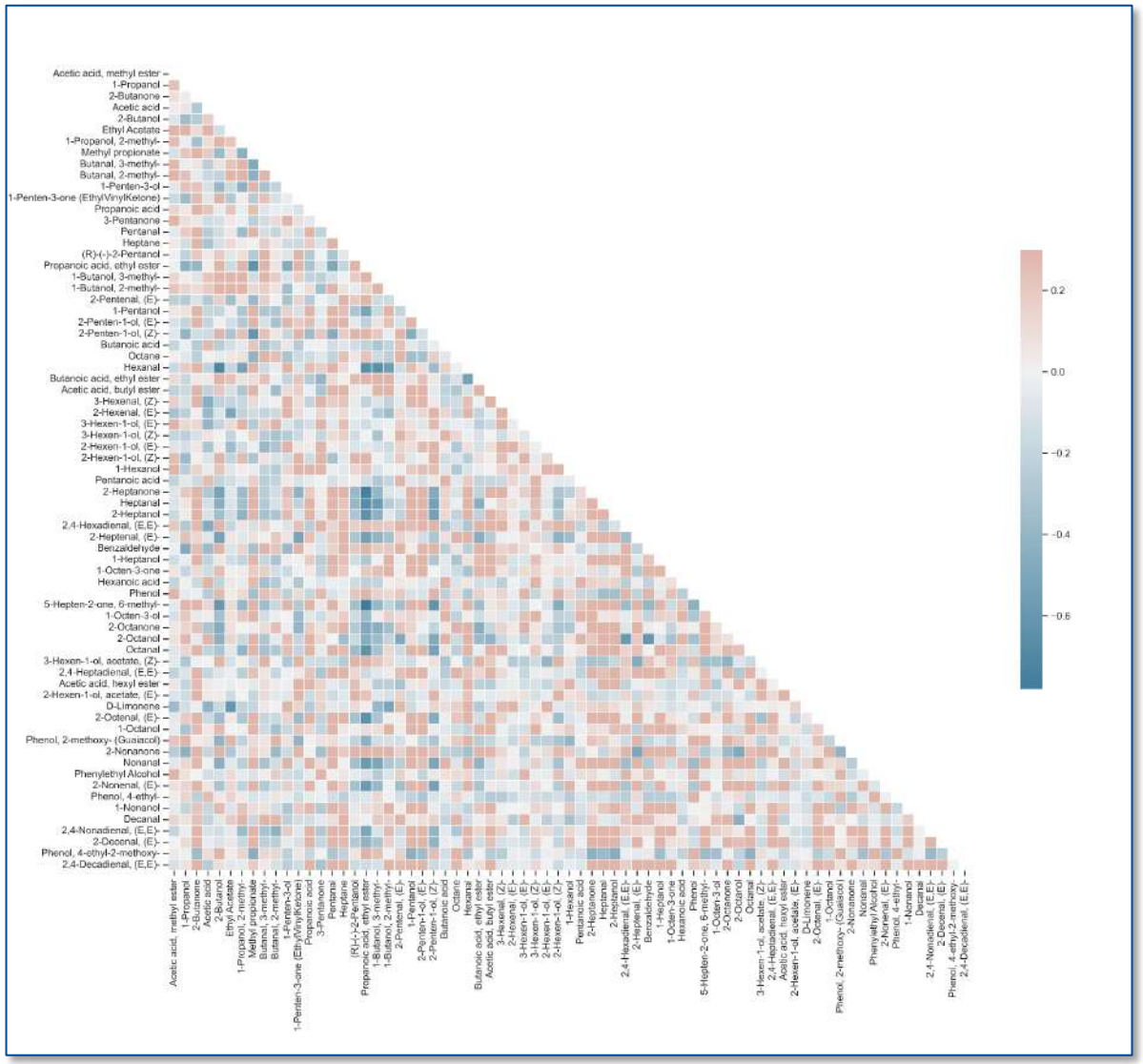
Chart: Odorous molecules.

OPERATIVE STEPS

1. Preprocessing data
2. Correlations
3. Visualization (dimension reduction)
4. Selection of the machine learning algorithm
5. Implementation of the machine learning process
    a. Preprocessing data: SMOTE/standardization (Standardscaler)
    b. Training
    c. Testing
    d. Validation
6. Deployment of the model

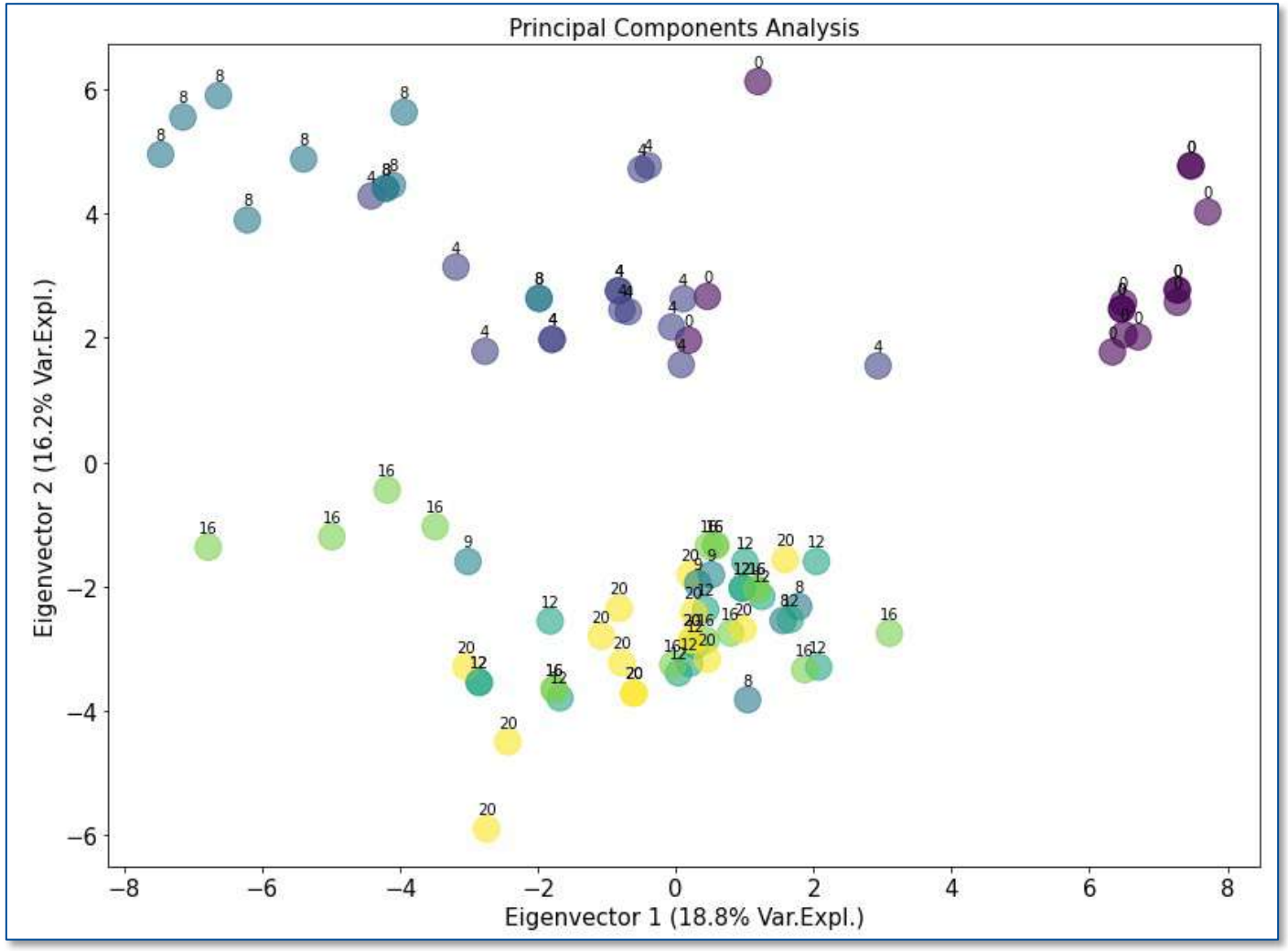


DESCRIPTIONS CORRELATIONS



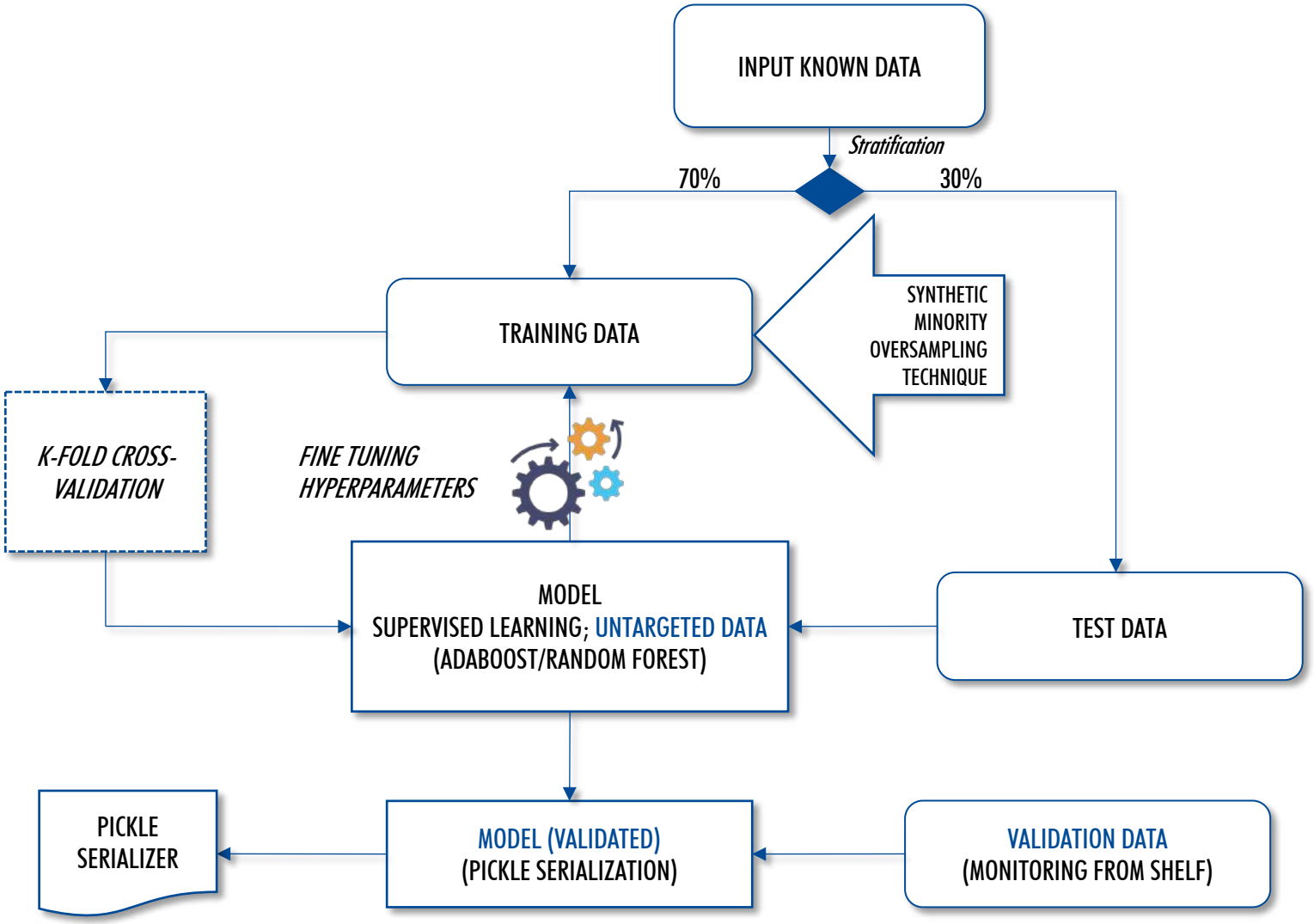
Scatterplot Correlation Matrix (Pearson coefficient).

PCA VISUALIZATION



Scatterplot Principal Components Analysis - Projection of the training samples.

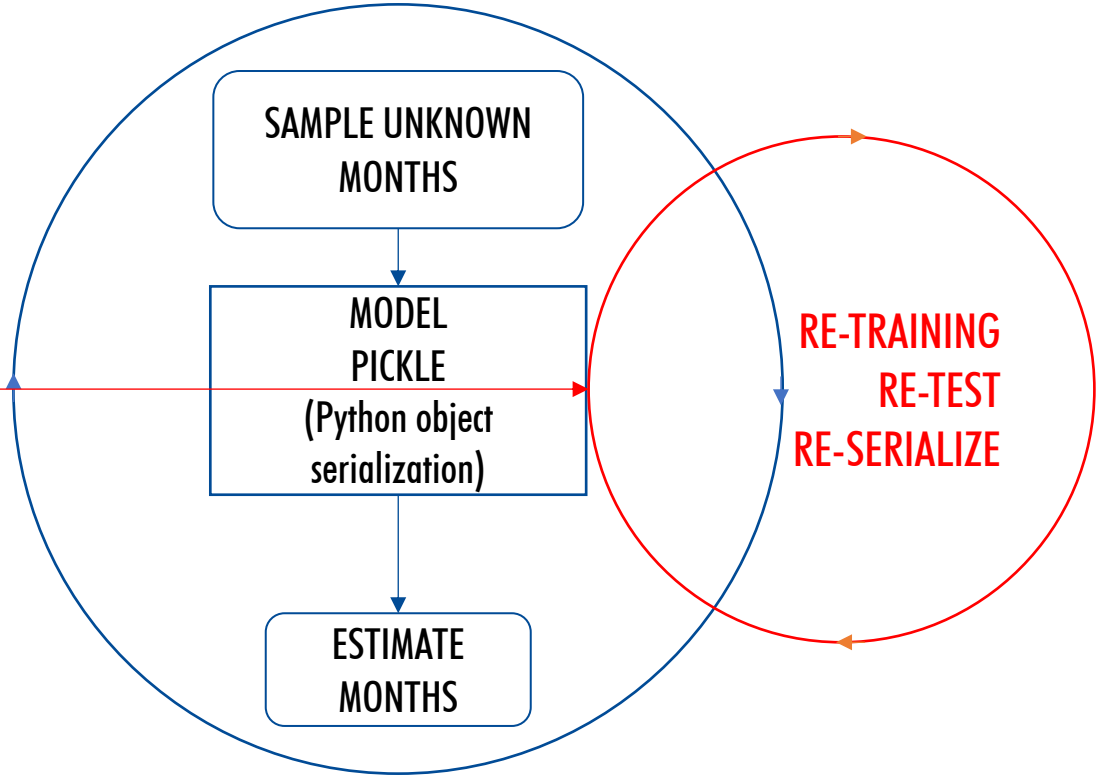
MACHINE LEARNING MODELING



CLOUD MODEL DEPLOYEMENT

IMPROVE
MODEL PERFORMANCE

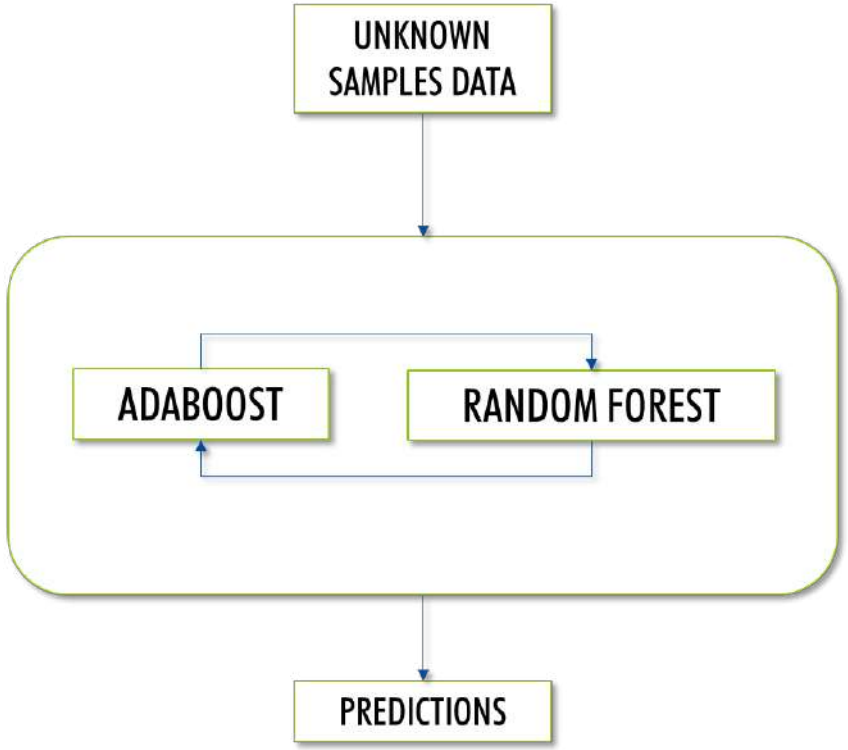
DATA BOOST:
MONITORING FROM SHELF
(30%)



MODEL PERFORMANCE

Performance Adaboost	
Coefficient of determination train	0,991
Coefficient of determination test	0,943
Mean absolute error train	0,342
Mean absolute error test	0,922

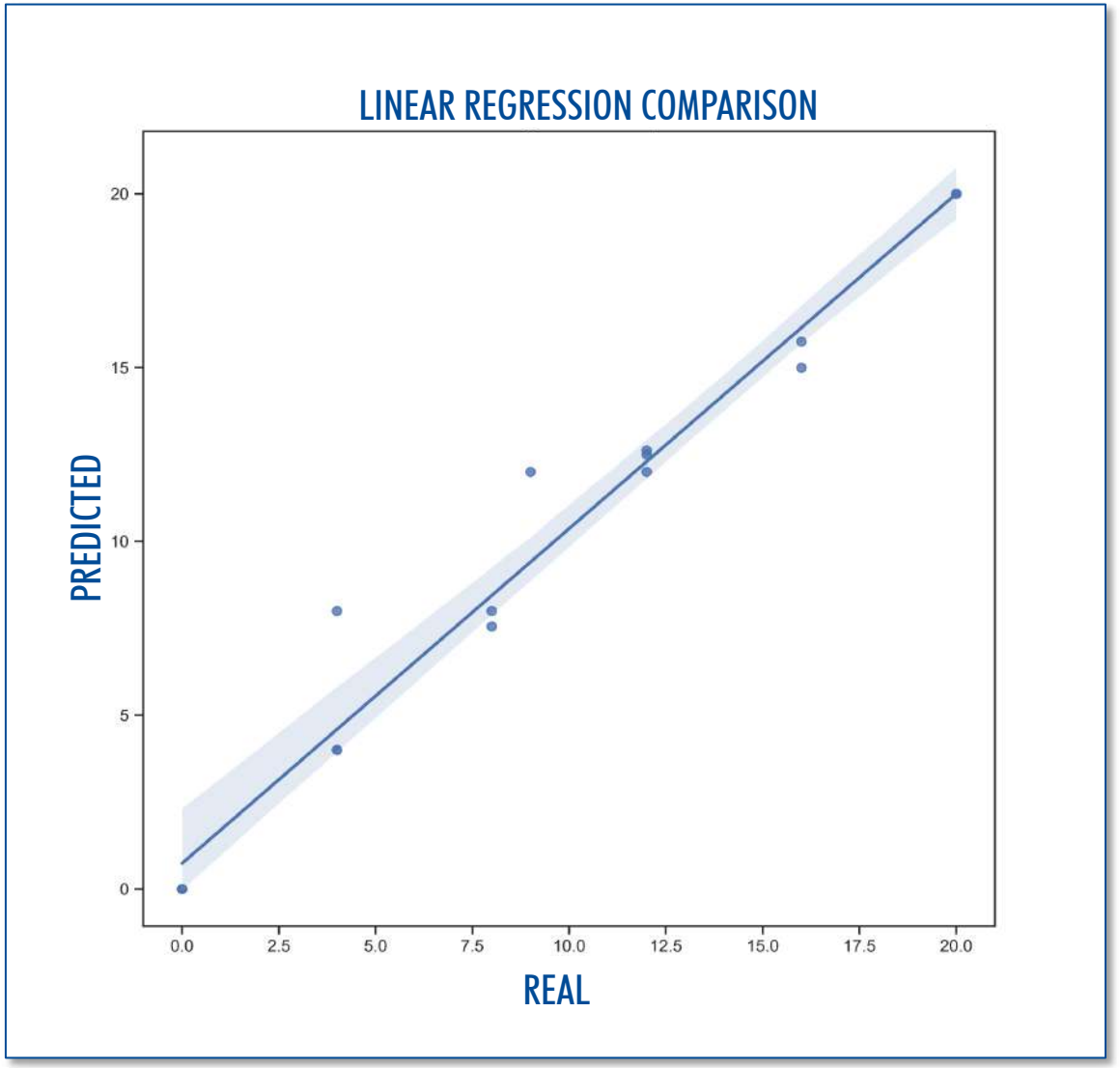
Performance Random Forest	
Coefficient of determination train	0,985
Coefficient of determination test	0,896
Mean absolute error train	0,684
Mean absolute error test	1,553



Category: Classification report (training) Random Forest				
	Precision	Recall	F-1 Score	Support
E	0.93	1.00	0.97	28
V	1.00	0.82	0.90	11
Accuracy			0.95	39
Macro avg	0.97	0.91	0.93	39
Weighted avg	0.97	0.95	0.95	39

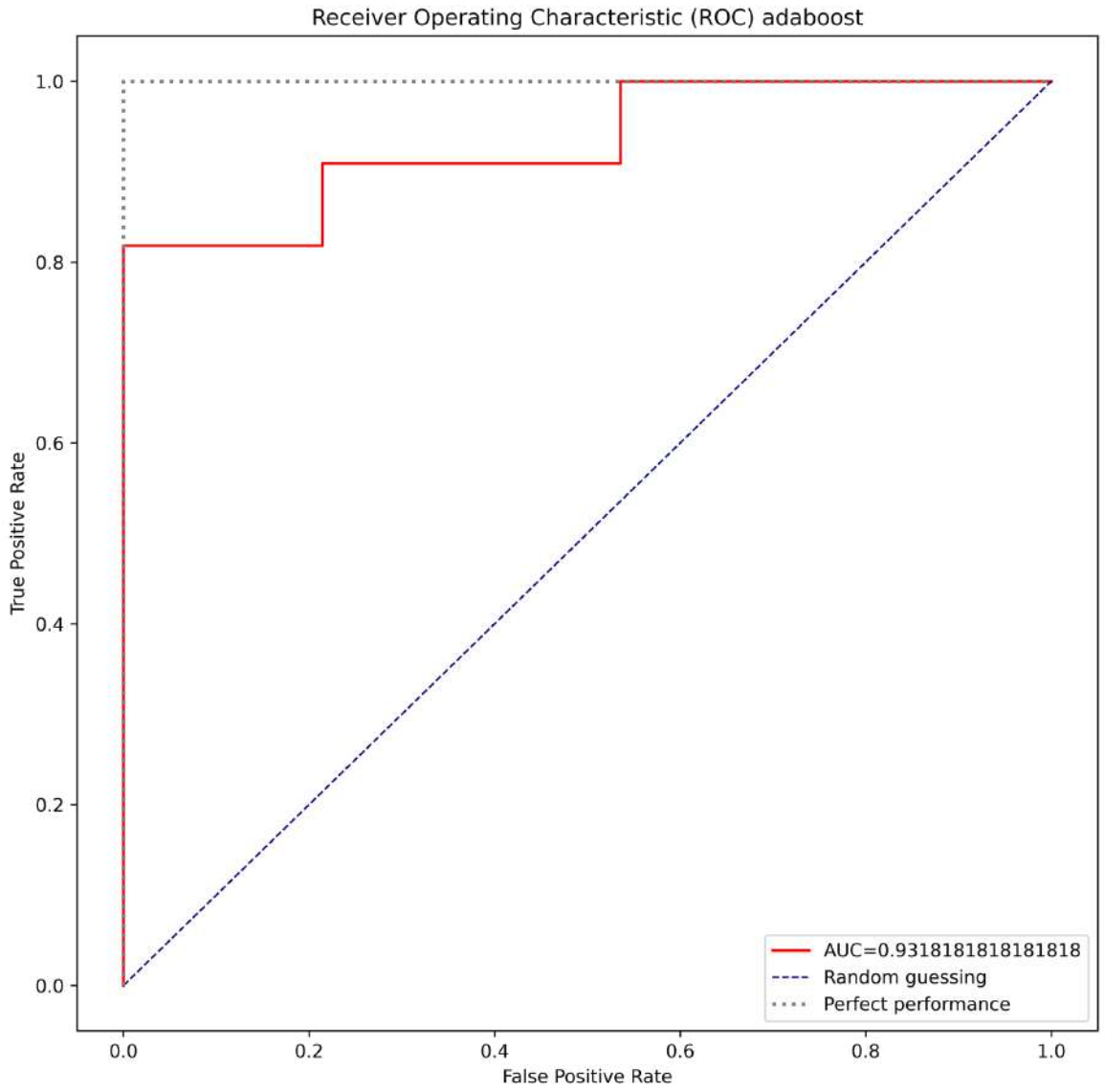
VALIDATION OF THE MODEL

Linear regression performance index (Adaboost)	Value
Coefficient of determination (R^2)	0,97
Slope (angular coefficient)	1,00
Intercept	-0,41
Root-mean-square error (RMSE)	1,29
Mean-square-error (MSE)	1,68
Mean-absolute error (MAE)	0,61



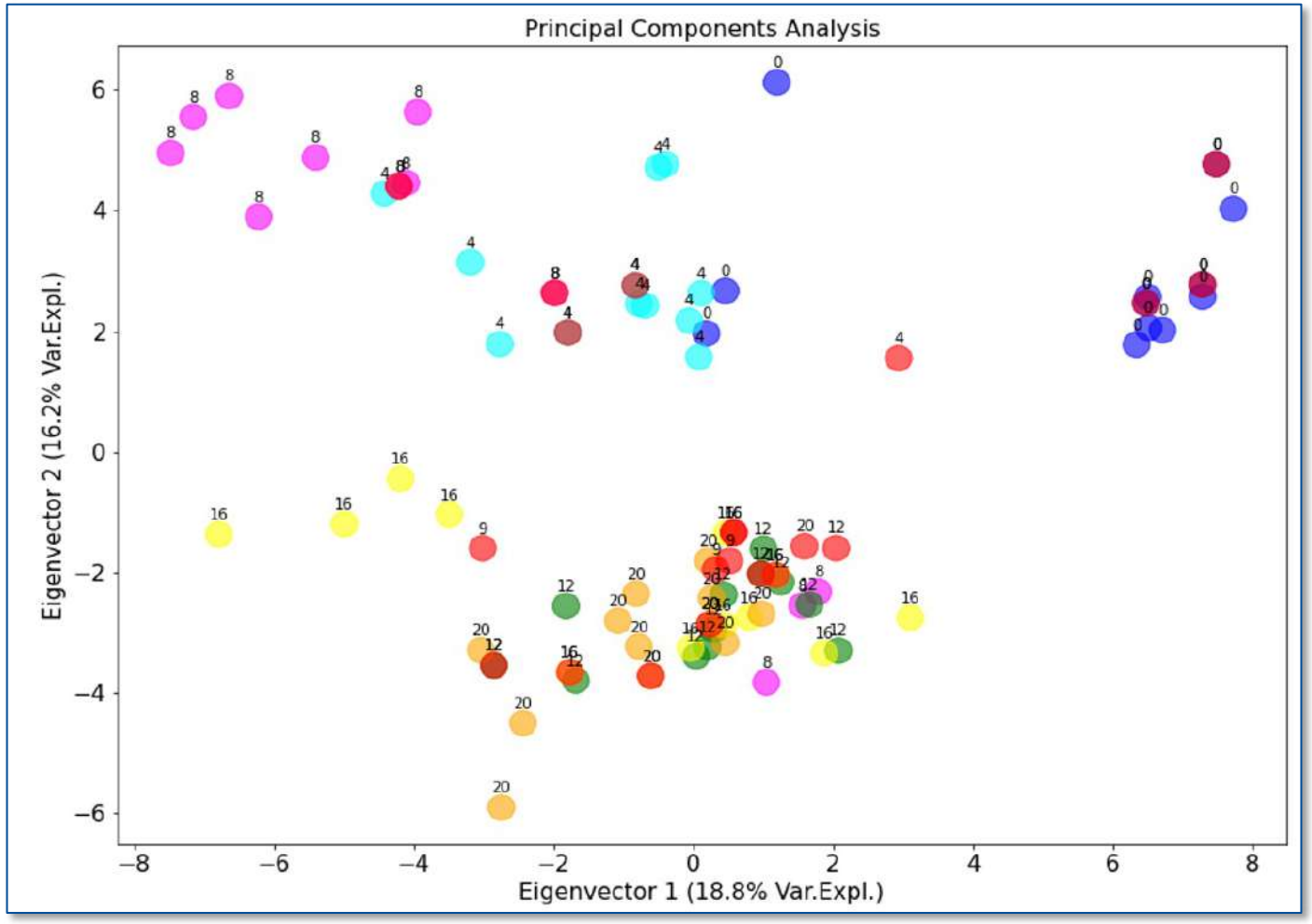
Scatterplot Linear Regression Model (real months versus predicted months).

VALIDATION OF THE MODEL



Real months	Predicted month	Real category	Predicted category
0	0	E	E
0	0	E	E
0	0	E	E
4	8	E	E
4	4	E	E
4	4	E	E
8	8	E	E
8	8	E	E
9	12	V	V
12	12	E	E
12	12	V	E
12	12	E	E
16	15	E	E
16	16	E	V
20	20	V	V
20	20	E	E

VALIDATION OF THE MODEL



Scatterplot Principal Components Analysis. Projection of the training samples and the validation samples (in red).

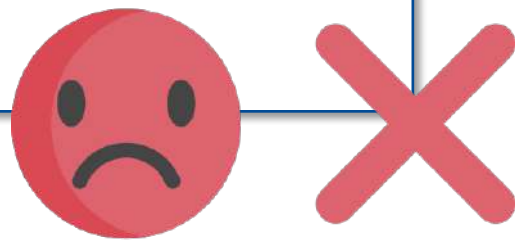
APPLICATION OF THE MODEL

APPLICATION N.1

Buying a sample of EVOO from the market at the time of the blend (batch).

- Months to end of shelf-life (EOSL) declared: 18
- Fitted months to EOSL by the model: 15
- Declared category at batch time: EVOO
- Fitted category at EOSL: VOO

Conclusions: must not buy this batch!

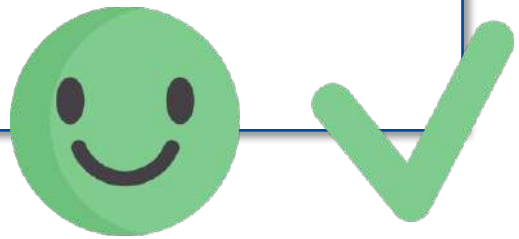


APPLICATION N.2

Monitoring from shelf: bottle of EVOO sampled at 12 months of shelf-life.

- Months to end of shelf-life (EOSL) declared: 6
- Fitted months to EOSL by the model: 12
- Declared category at batch time: EVOO
- Fitted category at EOSL: EVOO

Conclusions: this is a good batch!



SWOT ANALYSIS

STRENGHTS

The model is simple, effective, sustainable, spreadable.

WEAKNESSES

HS-SPME-GC/MS is a methodology that has some risk in reproducibility, which is however mitigable.

THREATS

Limitations of application to the types of mass market oils.

OPPORTUNITIES

Great use potential thanks to its simplicity and precision expressed (monthly).


QUESTIONS
ANSWERS

Thank you

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