WORLDWIDE PERSPECTIVES ON GEOGRAPHICAL INDICATIONS

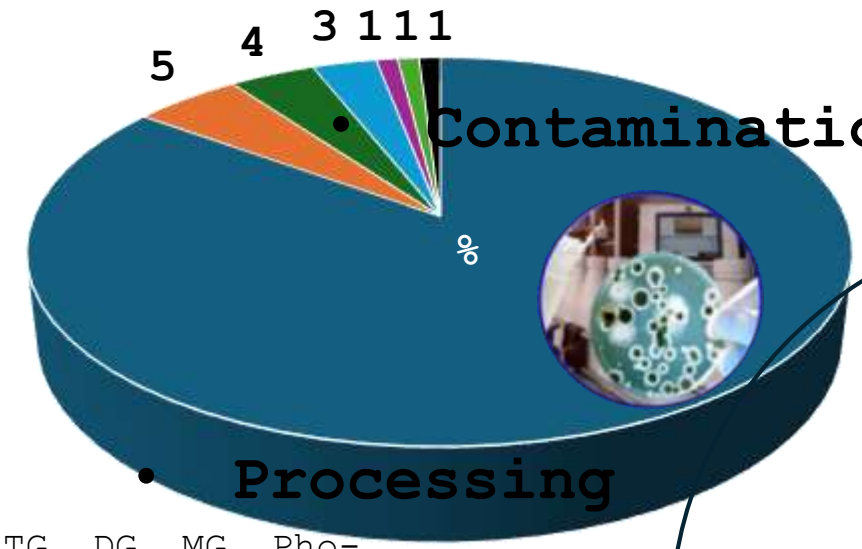
INTERNATIONAL CONFERENCE FOR RESEARCHERS, POLICY MAKERS AND PRACTITIONERS

INNOVATIONS AND TRADITIONS FOR SUSTAINABILITY

Gaia Meoni, Ph.D – CERM, Dipartimento di Chimica «Ugo Schiff», Università degli Studi di Firenze

Harnessing NMR metabolomic fingerprinting for enhanced geographical identification and quality of milk and coffee

FOOD: A COMPLEX MATRIX



- Contamination
- Processing

Water
Lipids: TG, DG, MG, Pho-L, sterols, carotenoids, vit. A, D, E, K, FA
Carbohydrates: lactose, oligosacc, sialic ac.
Proteins: casein, whey p., aa
Organic acids: lactic ac., citric ac., formic ac., etc
Minerals: Ca, K, Mg, Na, Cl, P, S
Other: NPN

- Origin

- Genetics

- Nutrition/Diet/Stress

Water
Lipids: Caffeol, TG, FA
Carbohydrates: mannose, raffinose, fructose, glucose, melanoidins
Alkaloids: caffein, trigonelline
Proteins: aa
Organic acids: CGA, caffeic ac., quinic ac., malic ac., lactic ac.
Minerals: Ca, K, Mg, Fe
Other

- Health status

- Season

Analytical tecniques for food analyses

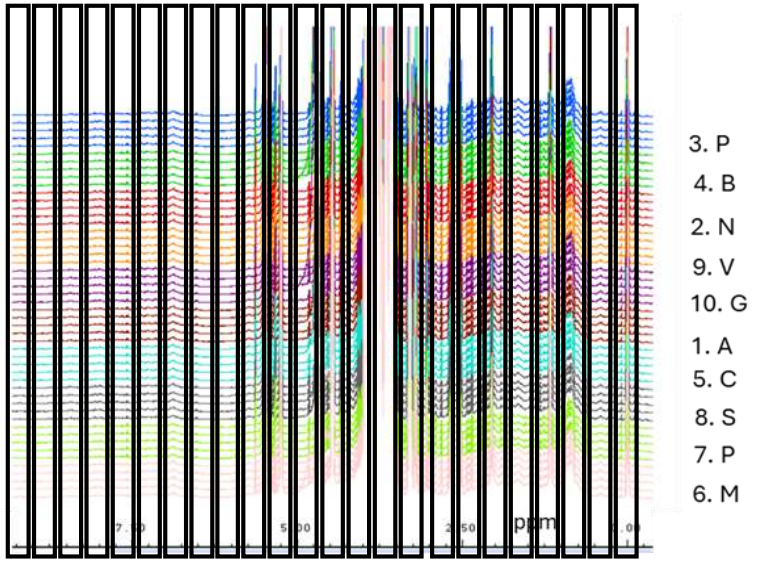
- ✓ Security
- ✓ Quality
- ✓ Authenticity

Common analyses :

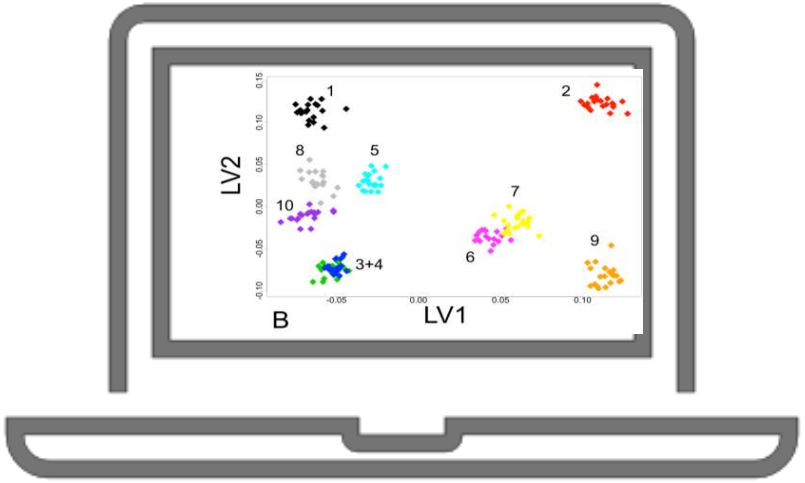
- Time consuming (low speed of detection, sample pretreatment)
- Sample distruction
- High volume/quantity of sample and solvents
- Targeted for few molecules

Fingerprinting analyses:

- Fast and minimal or no sample pre-treatment
- Non-destructive
- Untargeted



Database creation and modeling



^{1}H-NMR (Nuclear Magnetic Resonance)

- ✓ **Highly reproducible**
- ✓ **Quantitative analysis**
- ✓ **Fast analysis**
- ✓ **Not disruptive**
- ✓ **Simple and minimal sample preparation**
- ✓ **Sensitivity (detection limit in the order of µM)**

eographical origin: the milk case

2018

Contents lists available at ScienceDirect

Food Research International

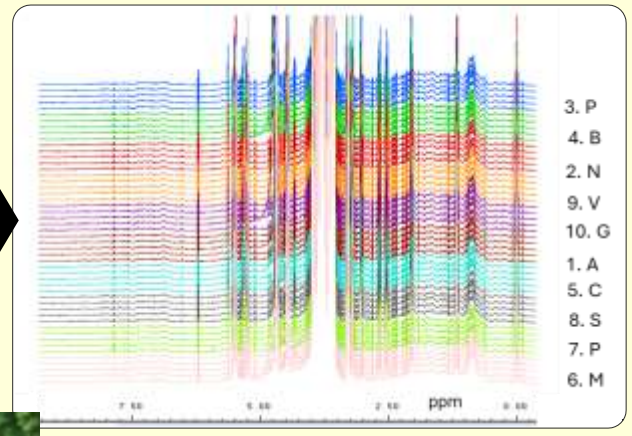
journal homepage: www.elsevier.com/locate/foodres

NMR metabolomic fingerprinting distinguishes milk from different farms

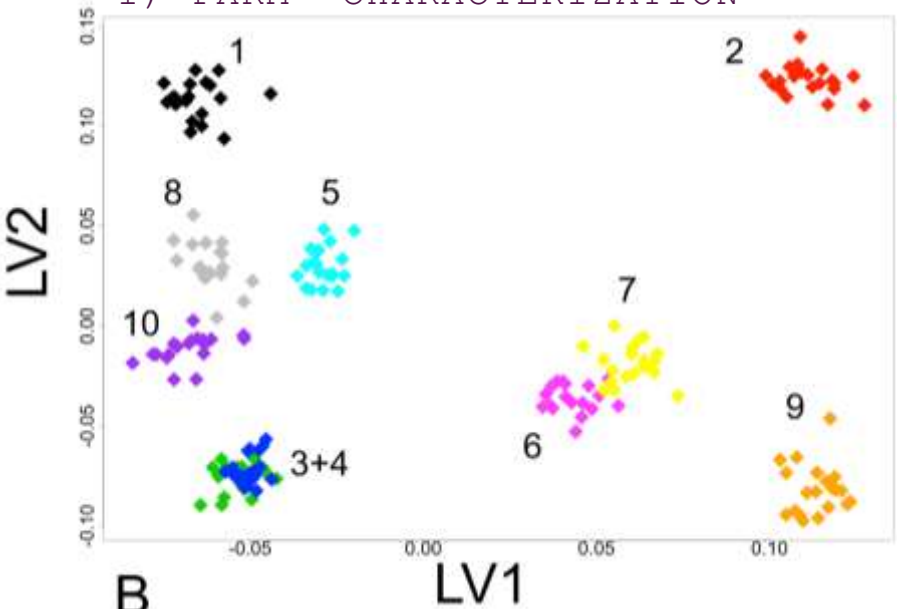
Leonardo Tenori[a,b], Claudio Santucci[b], Gaia Meoni[b], Valentina Morrocchi[c], Giacomo Matteucci[c], Claudio Luchinat[b,d,e,*]

400 raw milk samples from 10 Mugello's farms (20 samp./stab.)

- ^{1}H NMR SPECTRA



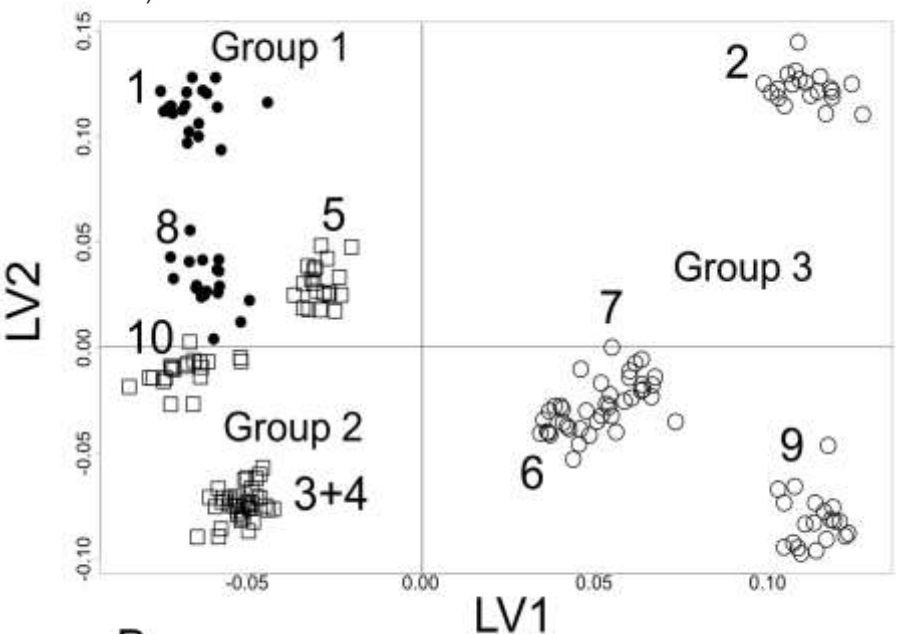
1) FARM CHARACTERIZATION



If 3 ≠ 4 ⇒ pred. acc **82%**

If 3 = 4 ⇒ pred. acc **97%**

2) CHARACTERIZATION OF THE FEEDING REGIMEN



- Group 1: silage and hays
- Group 2: silage
- Group 3: hays and cereal flour

↑ Hippurate, choline, methionine

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https://doi.org/10.3168/jds.2022-22072

Department of Agronomy, Food, Natural Resources, Animals and Environment (DAFNAE), UNIPD

Grazing affects metabolic pattern of individual cow milk

2022

G. Niero,[1] G. Meoni,[2,3] L. Tenori,[2,3] C. Luchinat,[2,3] G. Visentin,[4*] S. Callegaro,[5] E. Visentin,[1] M. Cassandro,[1,6] M. De Marchi,[1] and M. Penasa[1]

421 milk samples from 72animals

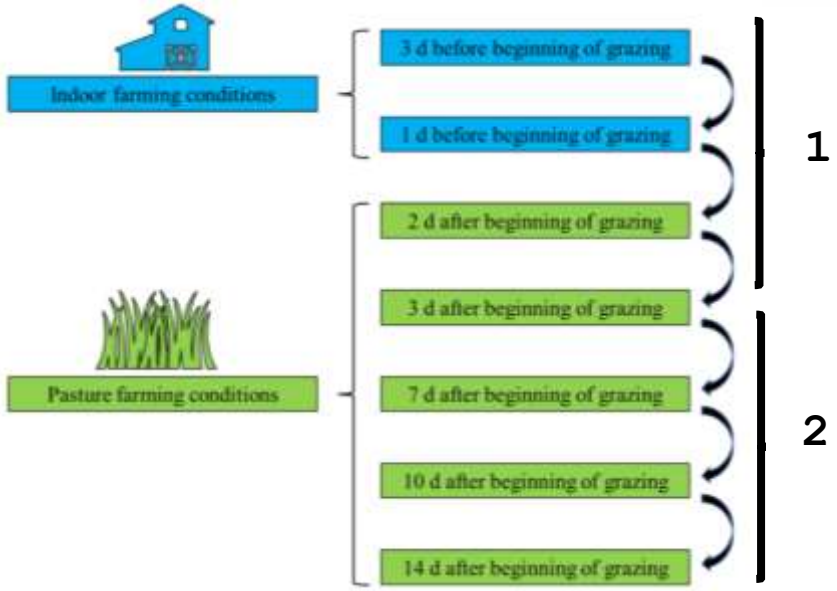


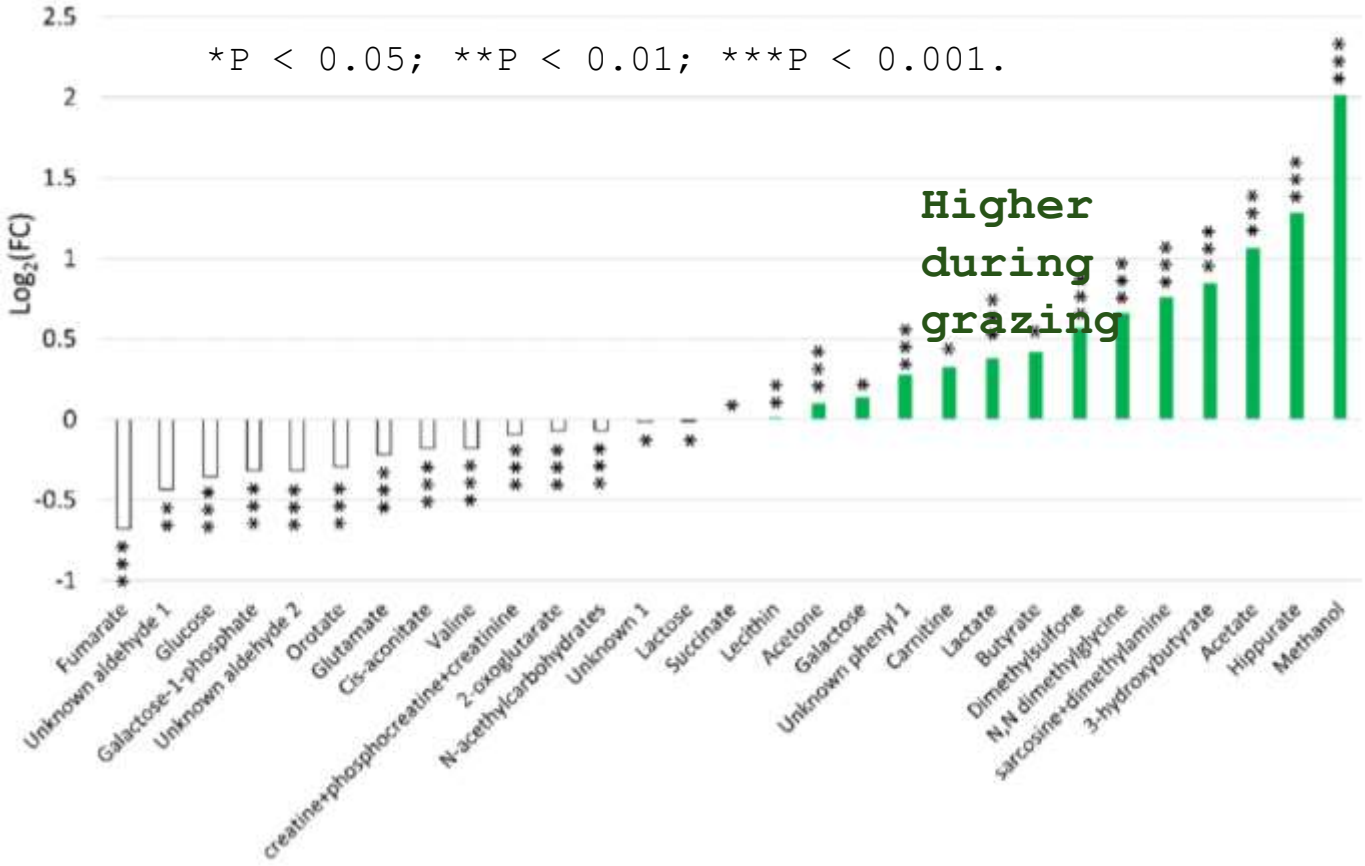
Table 2. Confusion matrix (%) of random forest model[1] built to classify different periods of sampling[2]

	Predicted period of sampling	
Actual period of sampling	1	2
1	97.6	2.4
2	12.9	87.1

[1]The diagonal of the confusion matrix reports the sensitivity (%) for the classification of each animal. Overall predictive accuracy = 93.1%.
[2]Period 1 refers to 3 and 1 d before the beginning of grazing and 2 and 3 d after the beginning of grazing; period 2 refers to 7, 10, and 14 d after the beginning of grazing.

uality and composition: the milk case

^{1}H NMR spectroscopy was used to investigate the effect of grazing on milk metabolites



- 93.1% accuracy distinguishing pre- and post-grazing milk samples.
- Hippurate: A robust marker for pasture-based milk.
- Grazing induces significant metabolic changes in milk.
- ^{1}H NMR is a powerful tool for food traceability and authenticity.
- Potential application in premium dairy product verification (e.g., PDO cheeses).

uality and composition: the milk case

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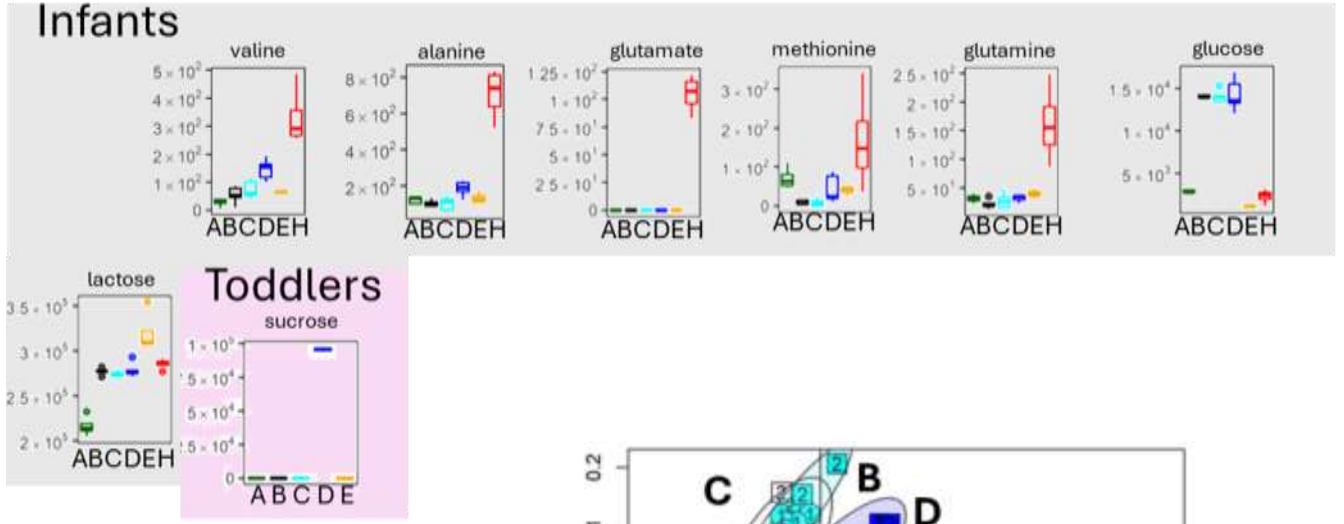
Research Article | NO ACCESS | Published Online: 6 July 2020

2020

Nuclear Magnetic Resonance-Based Metabolomic Comparison of Breast Milk and Organic and Traditional Formula Milk Brands for Infants and Toddlers

Authors: Gaia Meoni, Leonardo Tenori, and Claudio Luchinat | AUTHORS INFO & AFFILIATIONS

Publication: OMICS: A Journal of Integrative Biology • https://doi.org/10.1089/omi.2019.0125



OPLS-DA

1) Org. Vs conv. FMs CV OPLS-DS

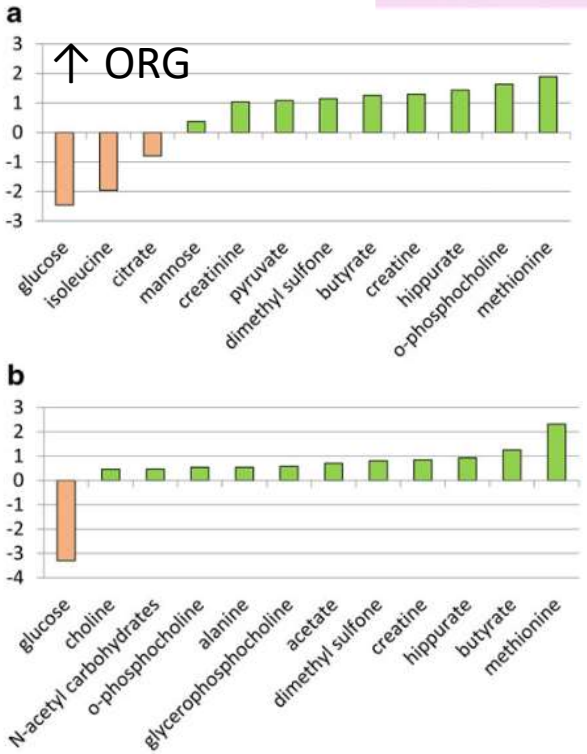
Confusion matrices of OPLS-DA models of organic and nonorganic infant FM

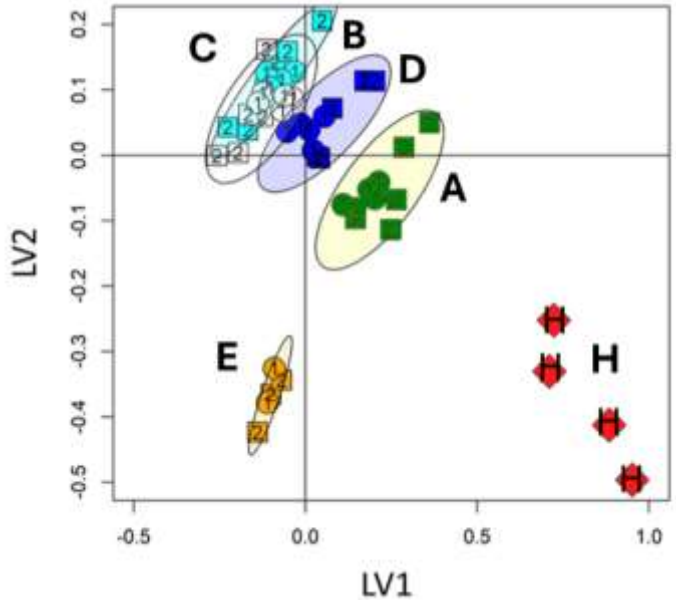
FM CPMG model			*FM diffusion-edited model*		
%	*NO-ORG*	*ORG*	%	*NO-ORG*	*ORG*
NO-ORG	66.7	33.3	NO-ORG	80	20
ORG	0	100	ORG	75	25
Overall predictive accuracy: 78%			Overall predictive accuracy: 61.6%		

2) 5 FMs CV OPLS-DS

%	*C*	*A*	*E*	*D*	*B*
C	20	0	0	0	80
A	0	100	0	0	0
E	0	0	100	0	0
D	0	0	0	100	0
B	70	0	0	0	30

Overall predictive accuracy: 70%





applied sciences 2021 MDPI

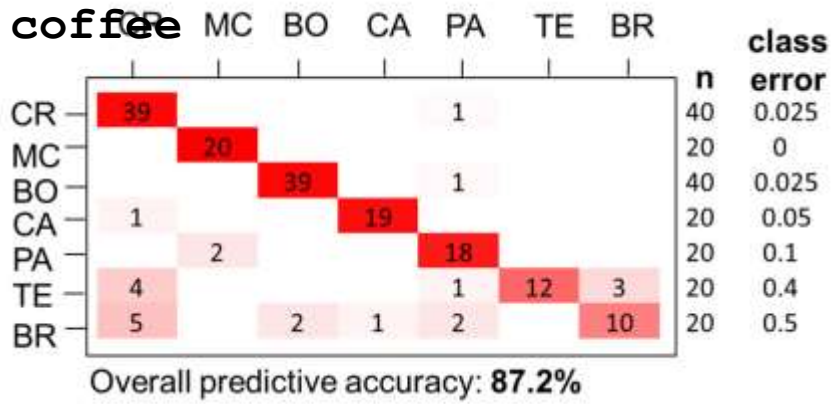
Article

Phenotyping Green and Roasted Beans of Nicaraguan Coffea Arabica Varieties Processed with Different Post-Harvest Practices & effect of processing: the coffee case

Gaia Meoni [1,2,3,*], Claudio Luchinat [1,2,3], Enrico Gotti [4], Alejandro Cadena [5] and Leonardo Tenori [1,2,3,*]

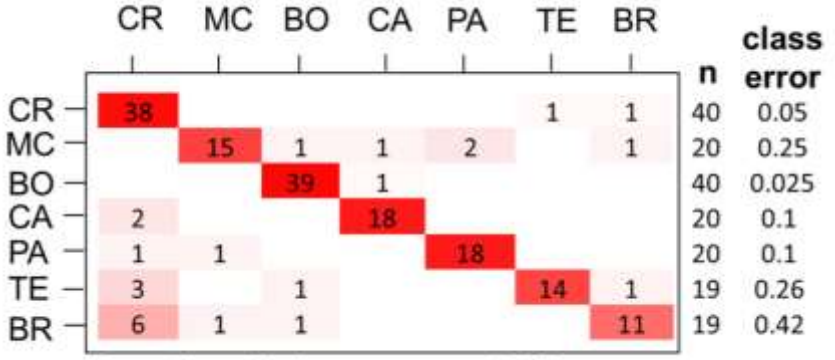
1) CULTIVAR CLASSIFICATION BASED ON ^{1}H-NMR FINGERPRINTING APPROACH

Green coffee

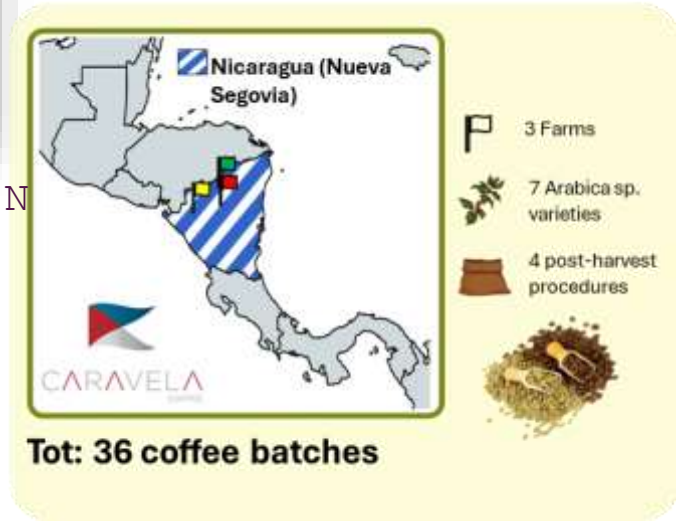


Overall predictive accuracy: **87.2%**

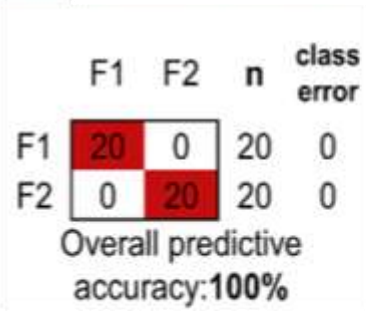
Roasted coffee

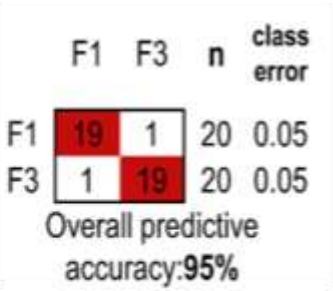


Overall predictive accuracy: **86%**



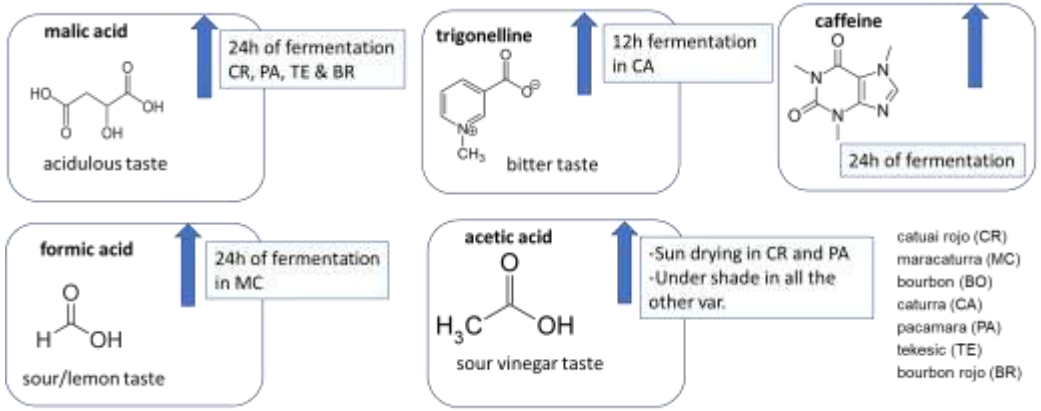
2) GEOGRAPHICAL CHARACTERIZATION OF NUEVA SEGOVIA FARMS CULTIVATING THE SAME VARIETIES





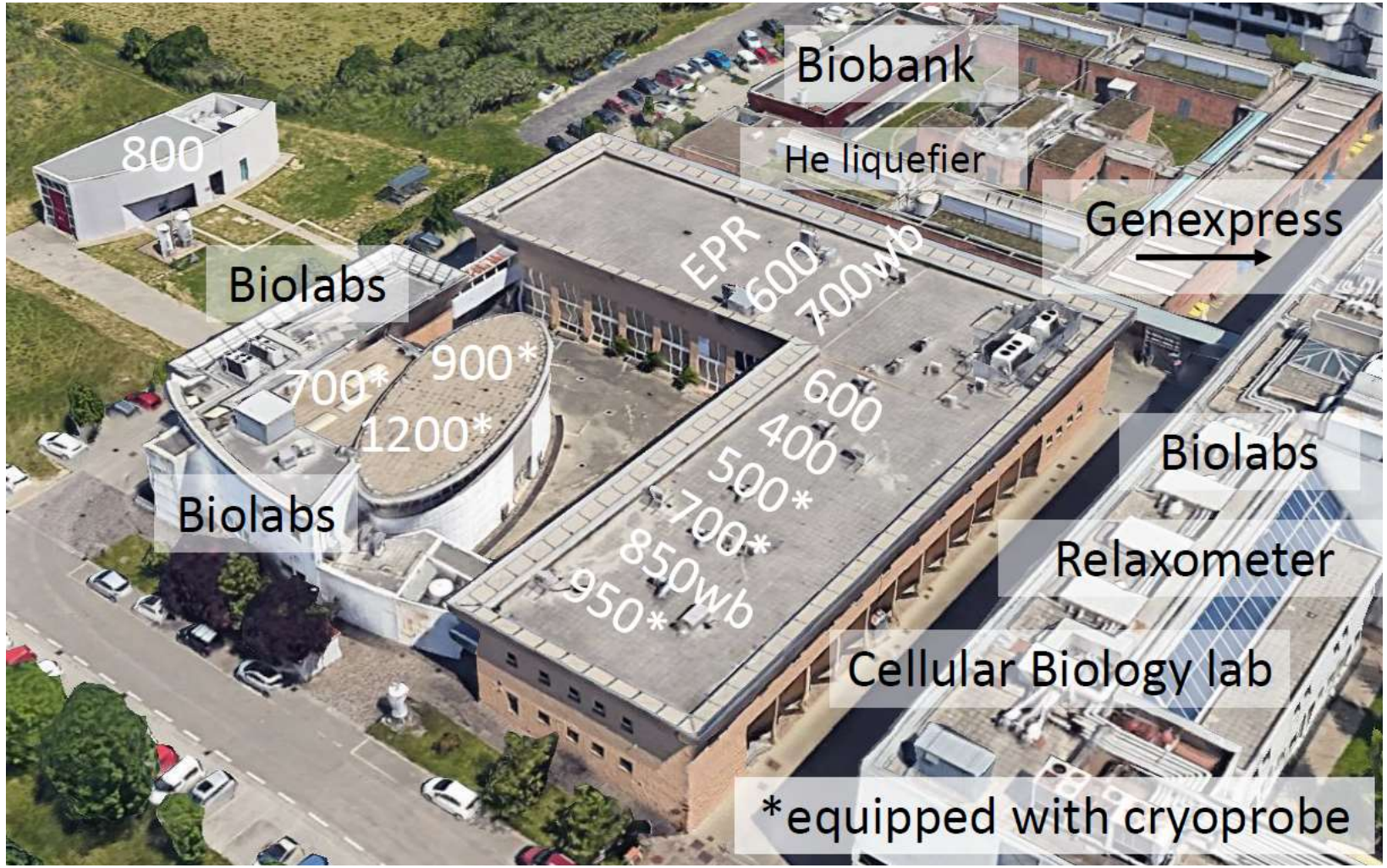
3) EVALUATION OF POST-HARVEST EFFECTS ON COFFEE METABOLOMIC PROFILE

catuai rojo (CR)
maracaturra (MC)
bourbon (BO)
caturra (CA)
pacamara (PA)
tekesic (TE)
bourbon rojo (BR)



- **Each coffee variety seems to react differently to fermentation, drying and roasting.**

MAGNETIC RESONANCE CENTER (CERM) @ UNIFI



CERM · CIRMMP INFRASTRUCTURE

Thank you for the attention