IDENTIFICAZIONE DI MISCELE ALIMENTARI MEDIANTE NMR

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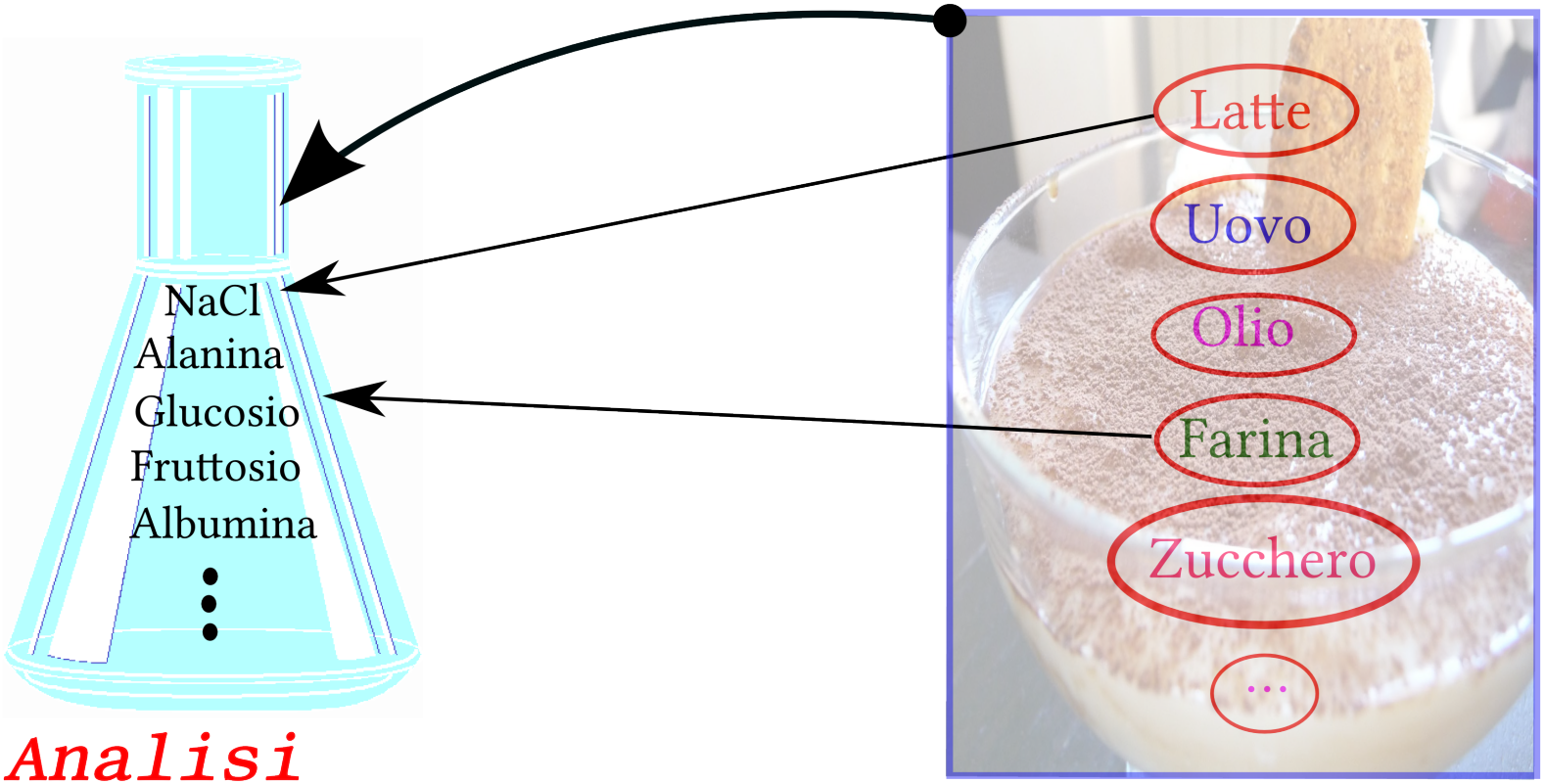
Miscele

Miscela chimica

(Gruppo di composti non interagenti)

Miscela alimentare

(Gruppo di ingredienti non interagenti)



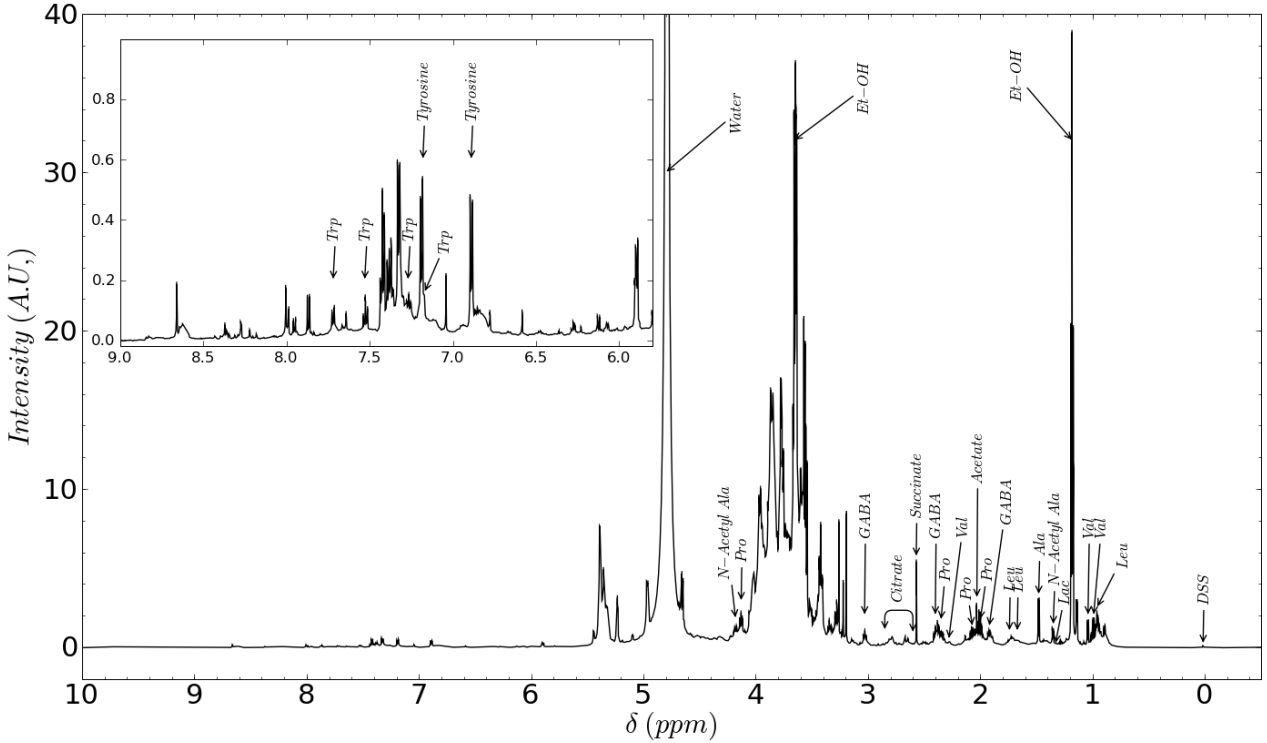
Analisi

Pattern Recognition

Identità chimica

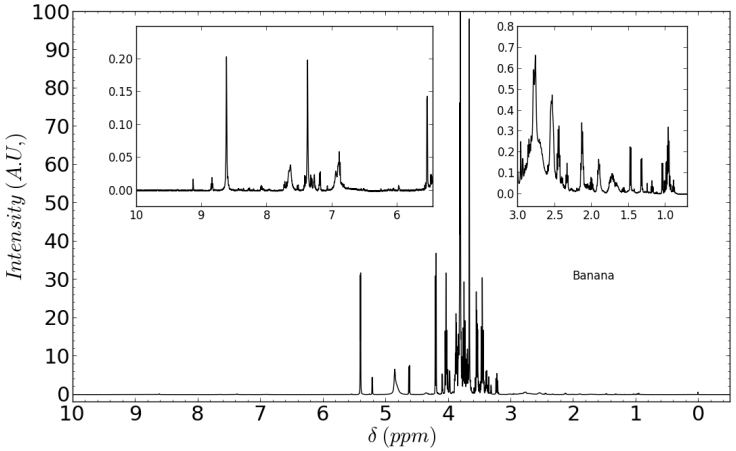
Cosa distingue da un punto di vista chimico un alimento da un'altro?

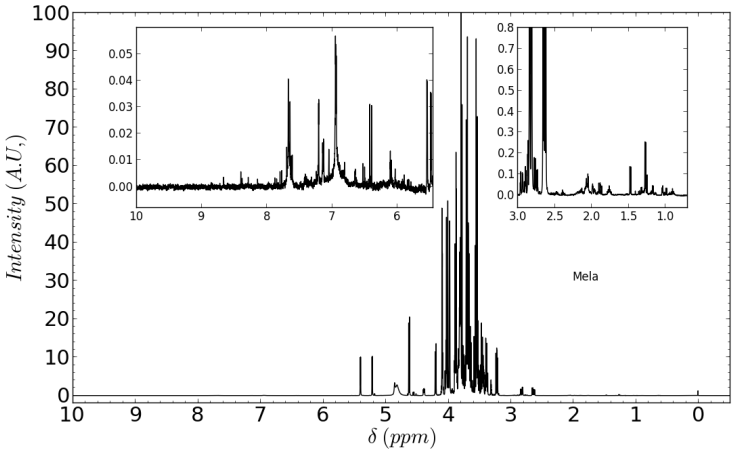
Pattern molecolari



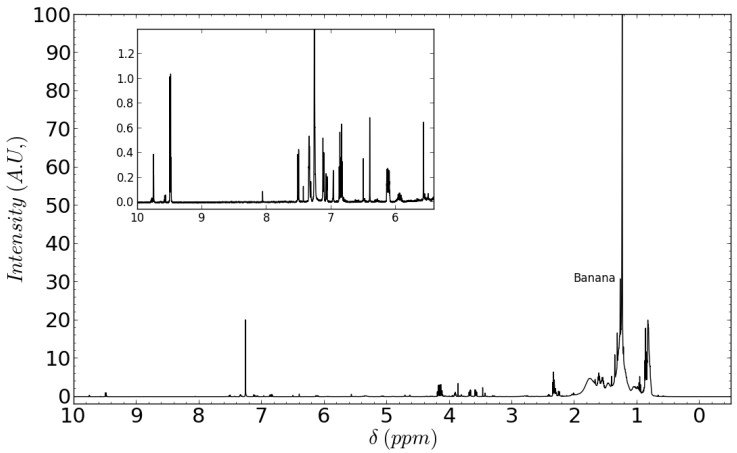
Profilo globale

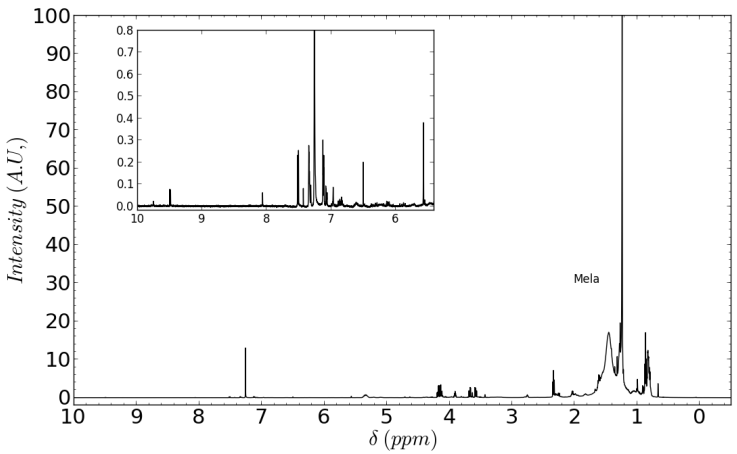
Fase acquosa





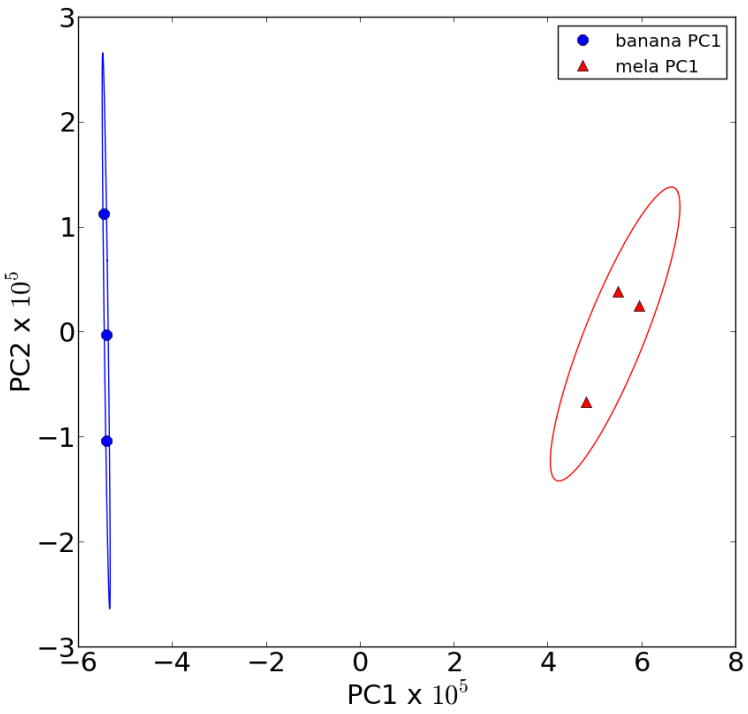
Fase Organica



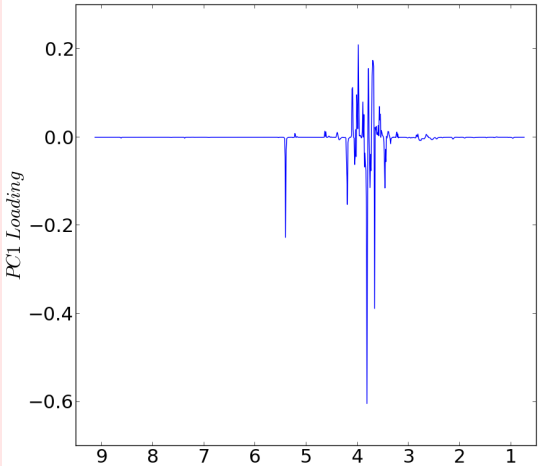


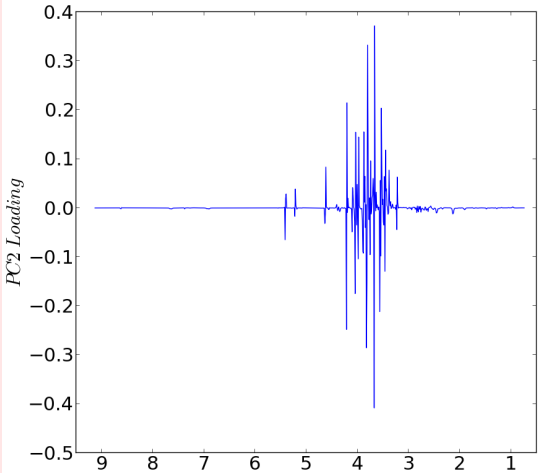
Variabilità naturale

PCA



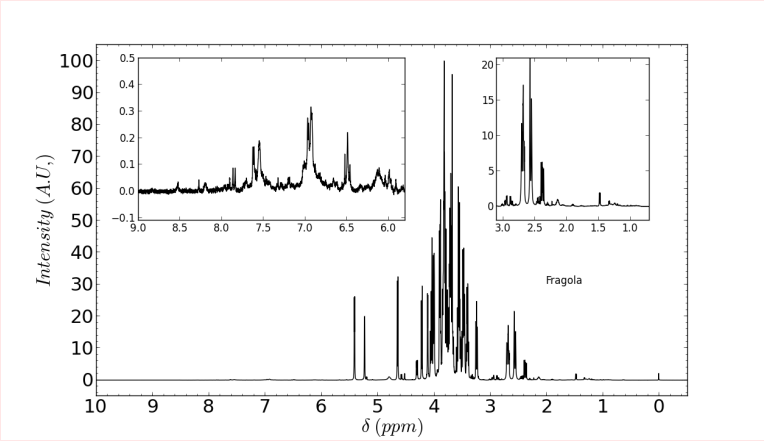
Loadings



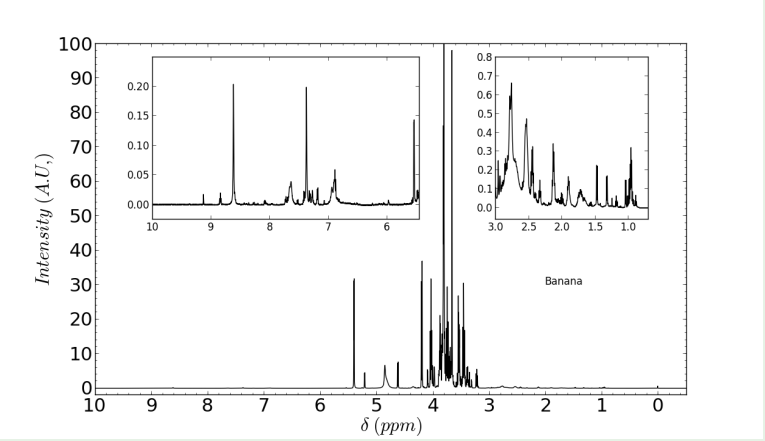


Quando vengono mescolati insieme gli ingredienti mantengono la loro identità chimica?

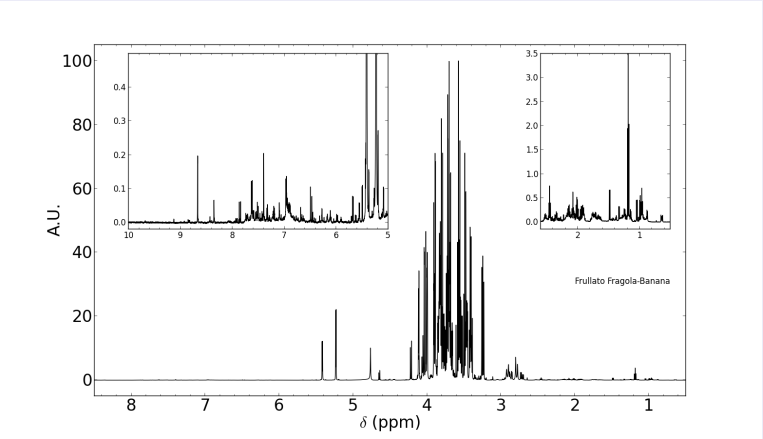
Fragola



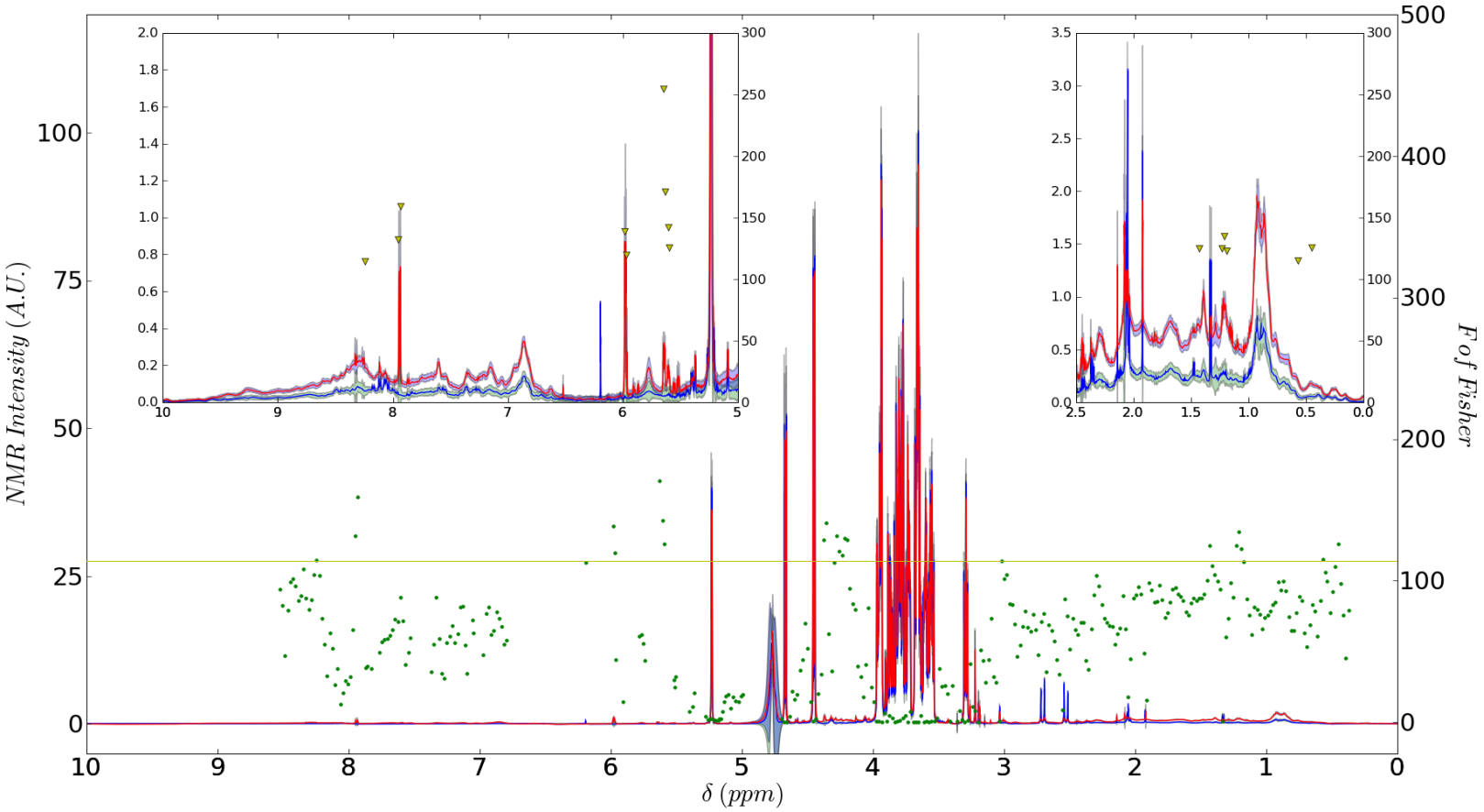
Banana



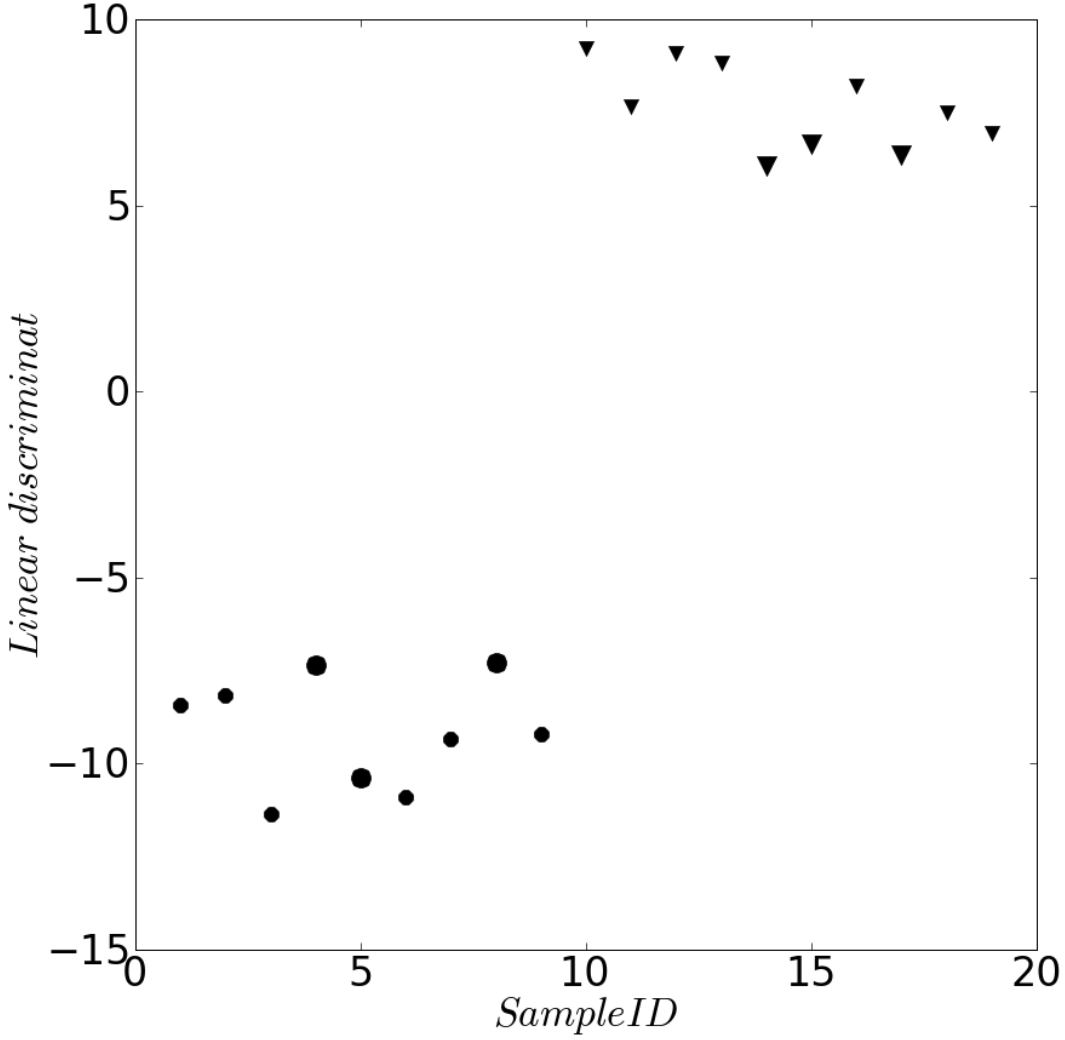
Frullato



Identità zoologica del latte (Mucca vs. Pecora)



LDA



Validazione

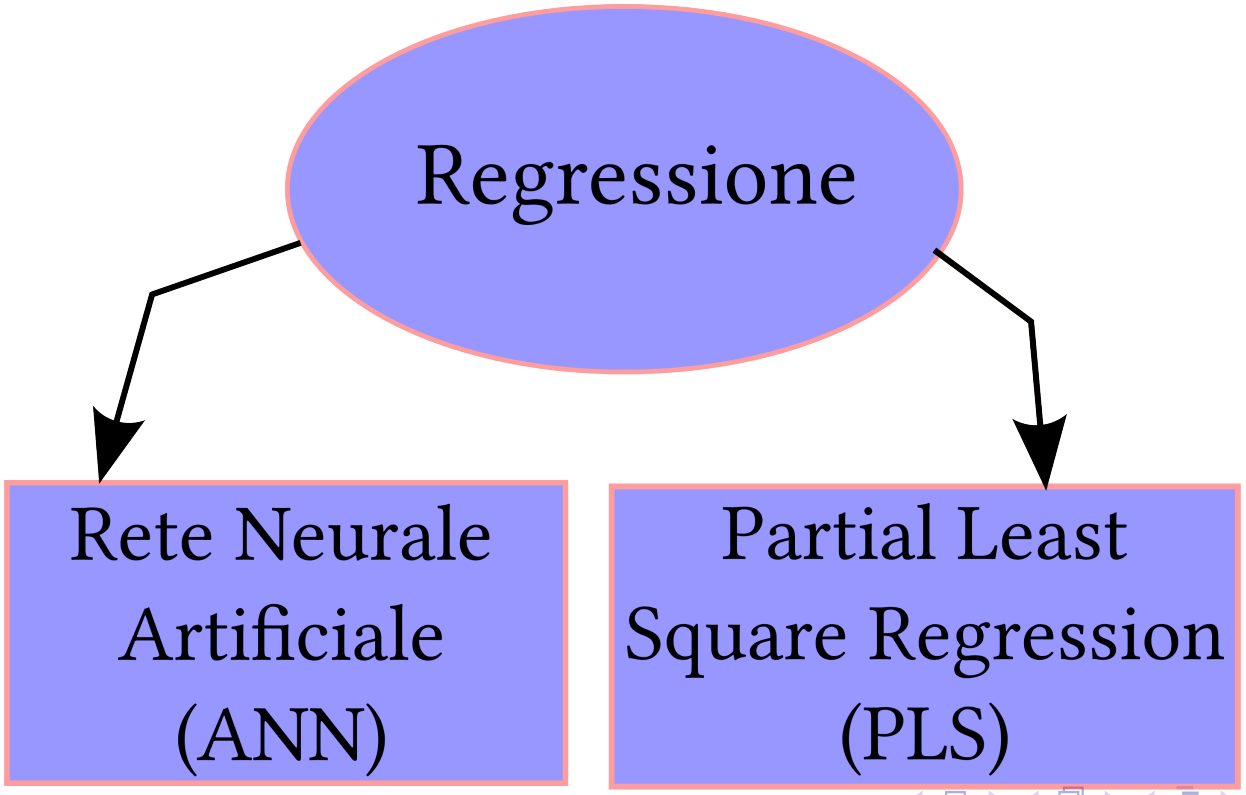
K-fold cross validation
100 %
K(3-9)

Quantificazione della miscela

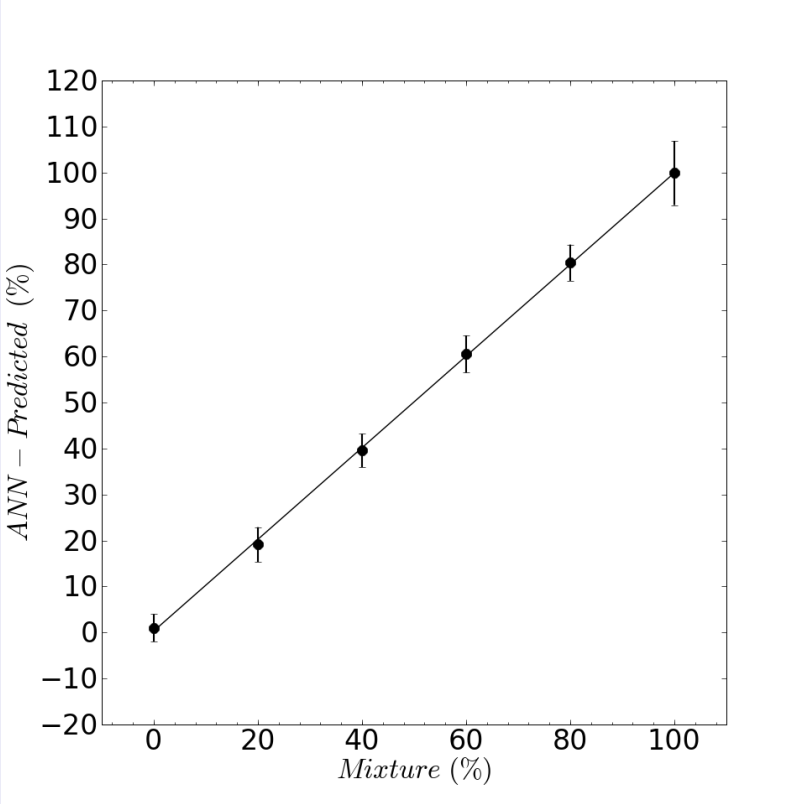
$$Y = BX + \epsilon$$
$$B = (X^t X)^{-1} X^t Y$$

Sorgenti di ridondanza

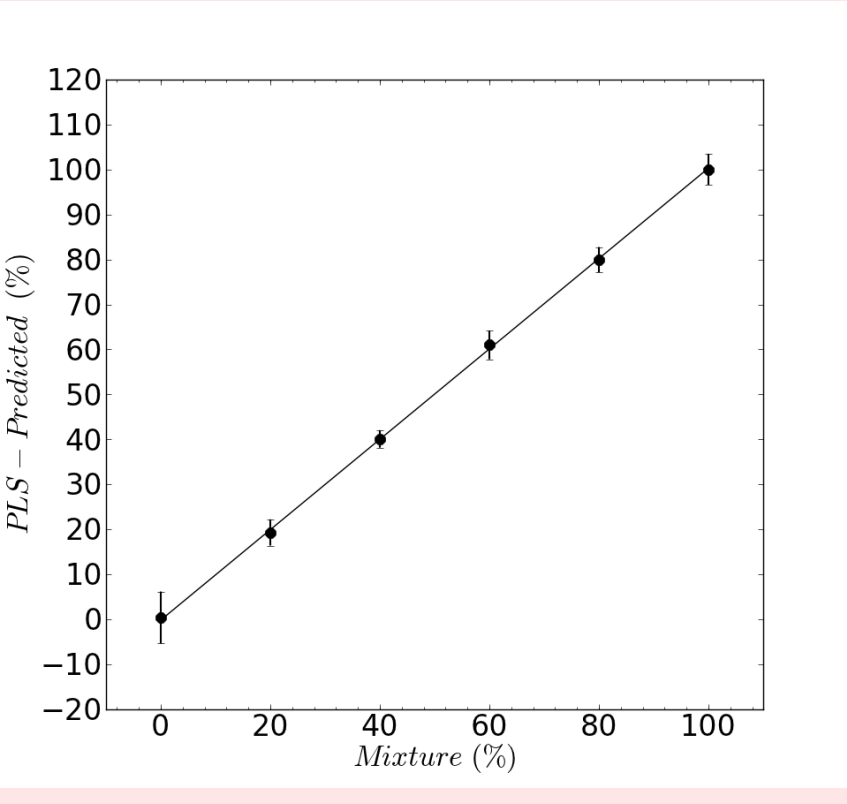
- Rumore chimico
- Correlazione fra le variabili



ANN

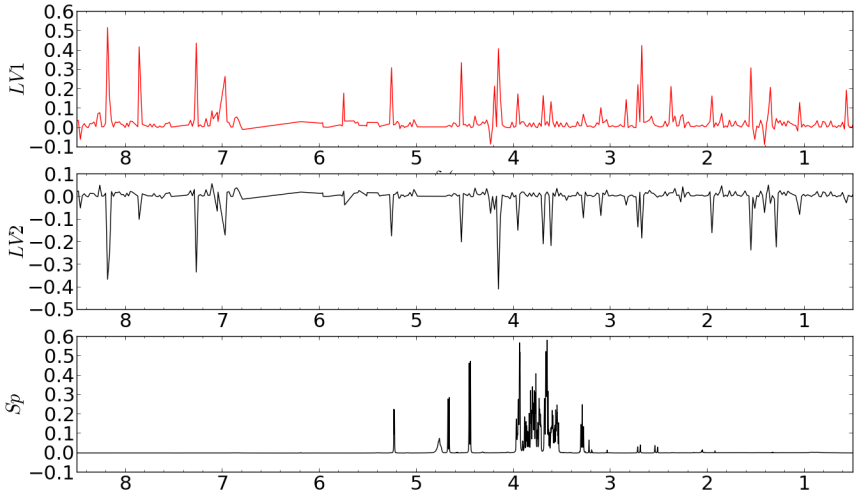


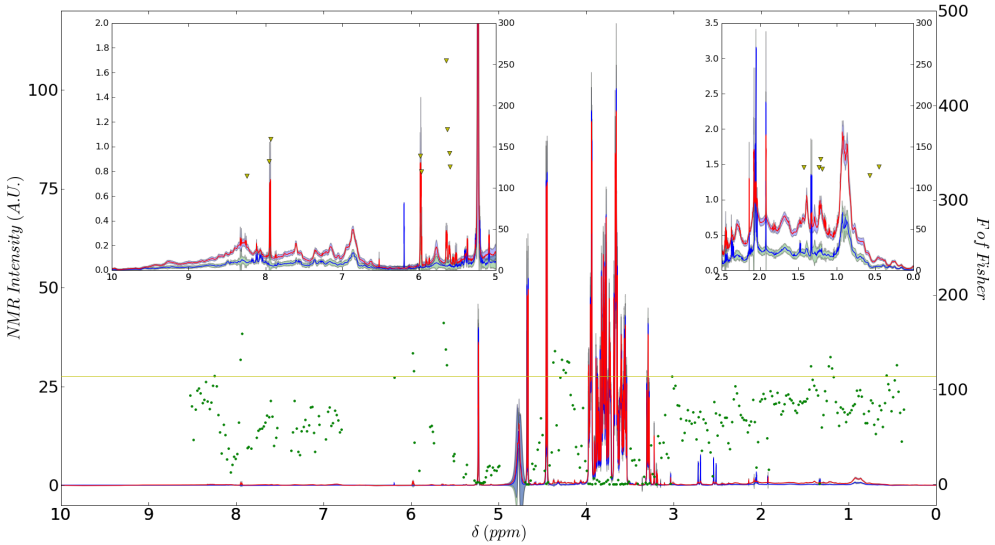
PLS



R. Lamanna, A. Braca, E. Di Paolo, and G. Imparato Magn. Reson. Chem. 49, S22-S26 (2012)

PLS Loadings





Miscele di Vini

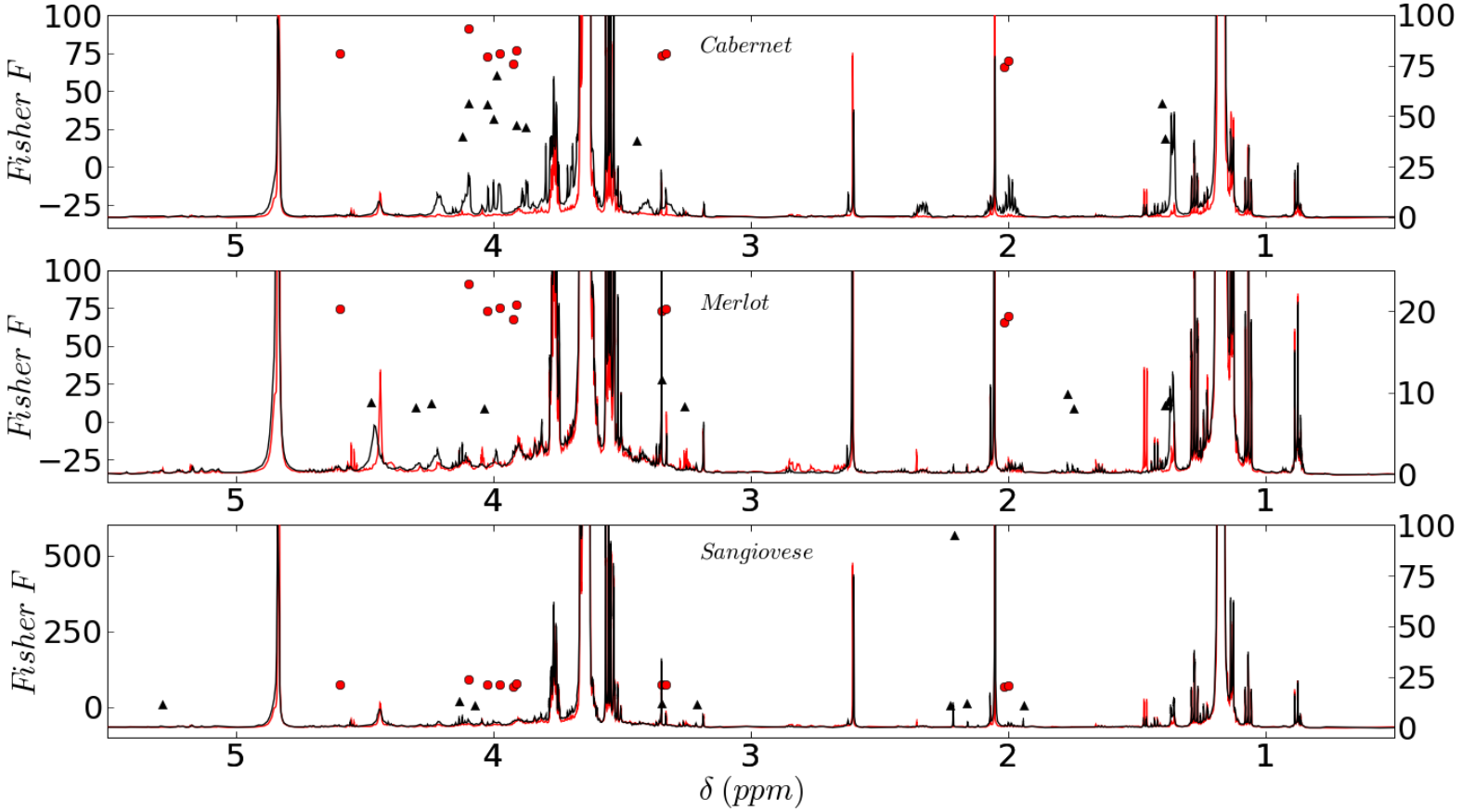
1. Montepulciano - Sangiovese
2. Montepulciano - Cabernet
3. Montepulciano - Merlot

Il problema delle miscele ha in realtà due gradi di complessità

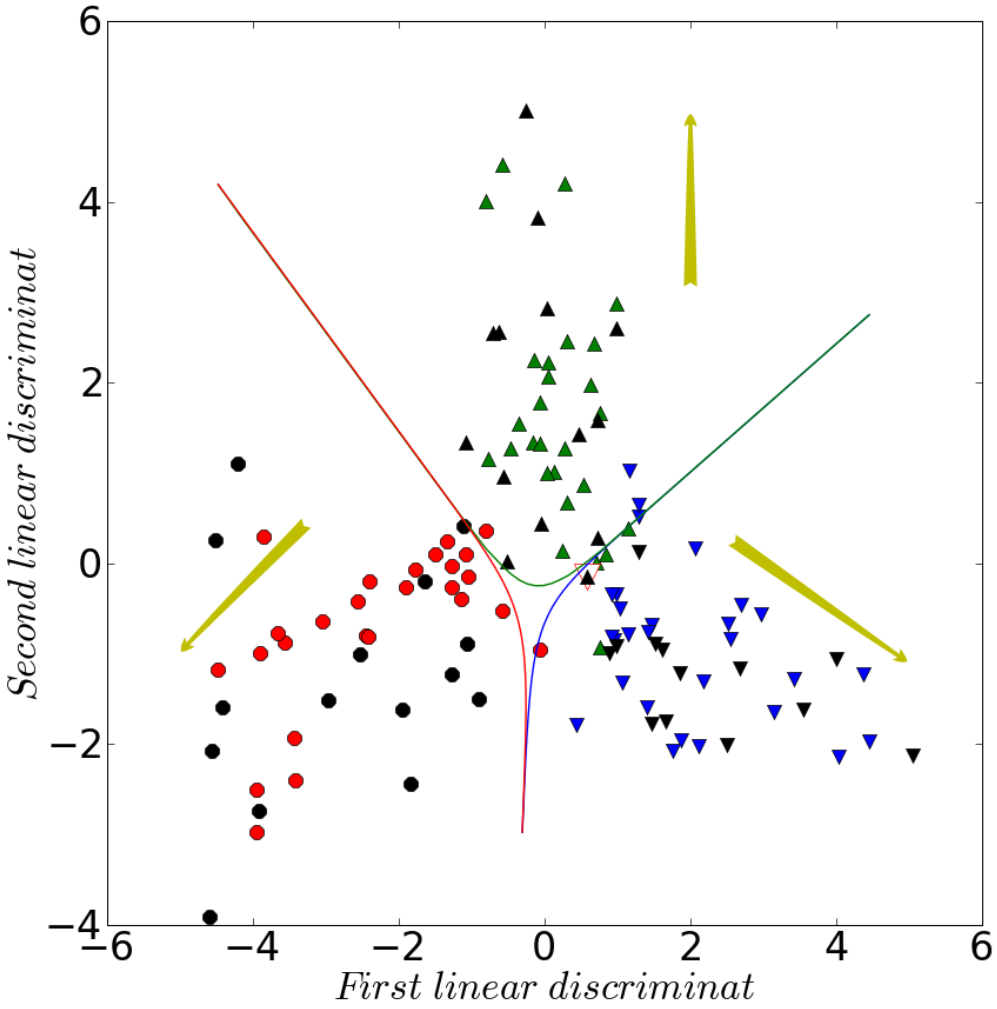
Individuare se il campione è una miscela e di che tipo.
(Classificazione)

Quantificare i componenti della miscela
(Regressione)

Selezione delle variabili per ogni grado di complessità.



Classificazione delle Miscele



Miscela Montepulciano-Sangiovese

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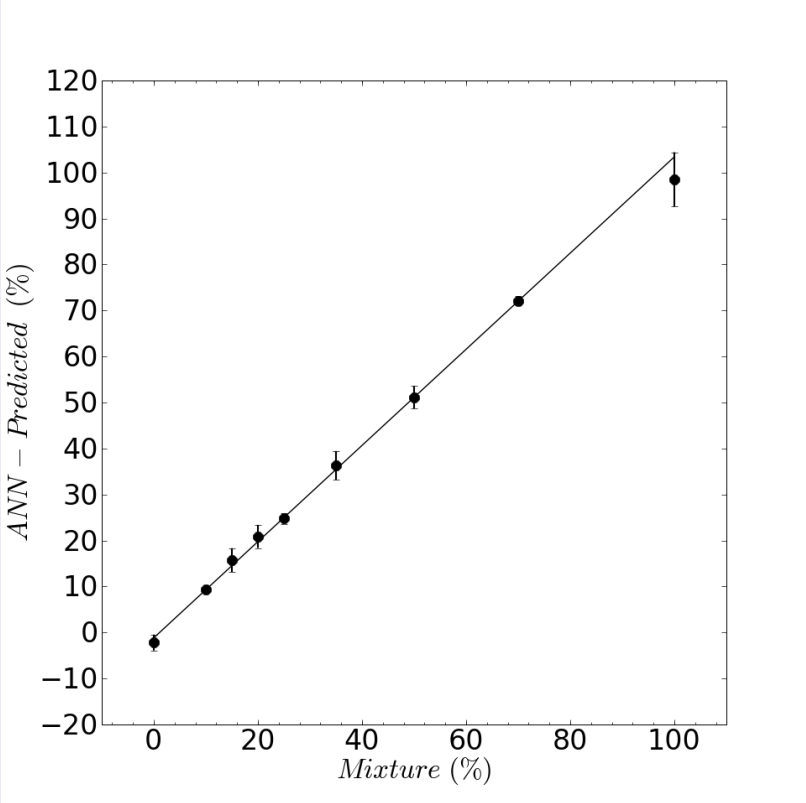
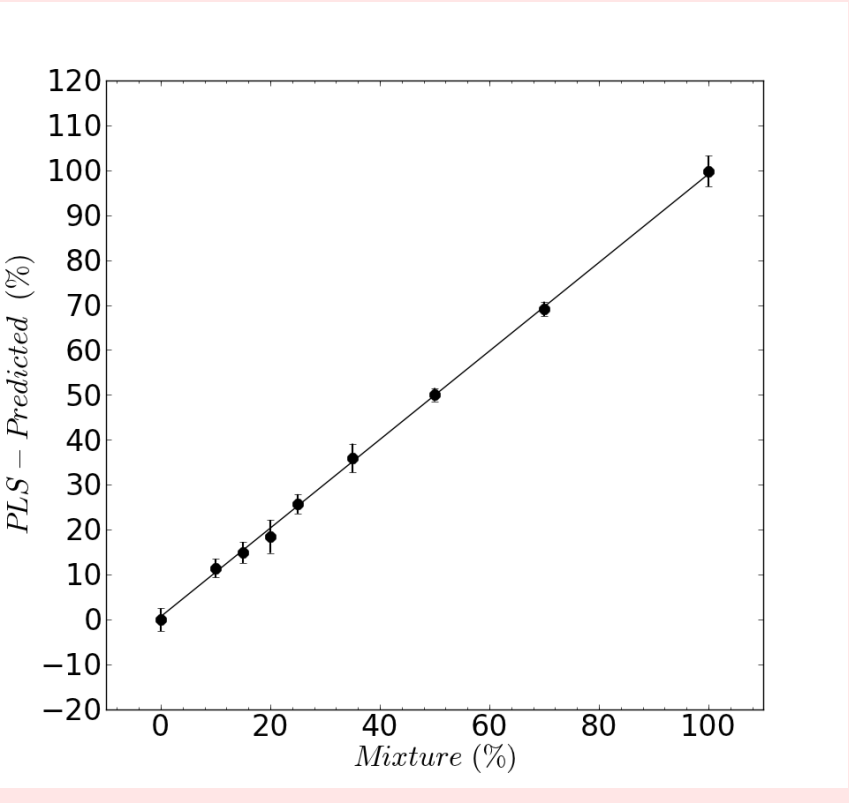
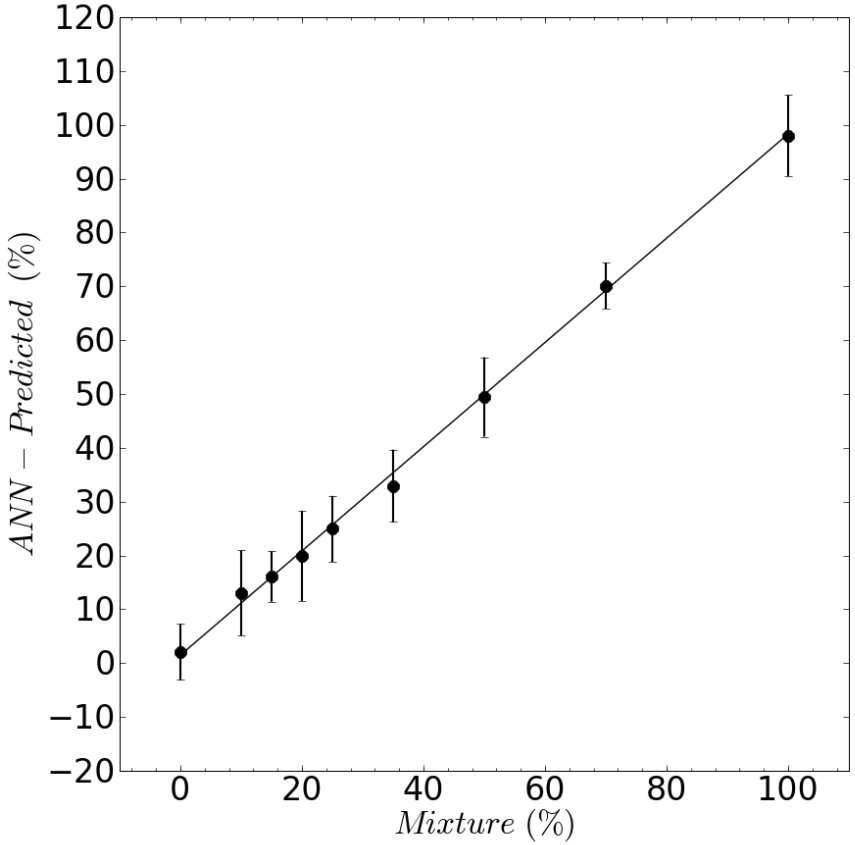


PLS



G. Imparato, E. Di Paolo, A. Braca and R. Lamanna J.Agric. Food Chem. 59, 4429-4434 (2011)

Montepulciano-(Sangiovese, Merlot, Cabernet)



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Conclusioni

- L'identificazione e quantificazione delle miscele alimentari è un problema di "pattern recognition" e non un semplice problema analitico.
- La NMR fornisce una rappresentazione molto ampia del profilo chimico di un alimento garantendo una più alta probabilità di trovare un schema adeguato per classificare e quantificare le miscele alimentari.
- La quantificazione di miscele alimentari richiede l'identificazione dello schema chimico di almeno uno degli ingredienti
- Il metodo che è stato applicato con successo all'identificazione e quantificazione di miscele di vini e latti apre la possibilità di identificare gli ingredienti di una miscela alimentare mediante l'uso del profiling chimico.

Questo lavoro è frutto di una collaborazione fra ENEA Trisaia e il COTIR di Vasto

Grazie a

Giavanna Imparato

Angela Braca

Elvio Di Paolo

e tutti voi !!