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HOW TO PREDICT THE ODOR PROFILE OF WINE FROM ITS CHEMICAL COMPOSITION ? IN SILICO MODELLING USING EXPERTS' KNOWLEDGE, FUZZY LOGIC AND OPTIMIZATION

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BACKGROUND

The odor component of food represents the identity, exemplarity, acceptability and the recognition by consumers of the food product¹

The analysis of food odor provides a list of molecules², but no information about the perceptual influence of mixed compounds

The perception of a mixture of odorants is not the simple sum of the odor of each odorants but the results of highly complex perceptual interactions^{3,4}

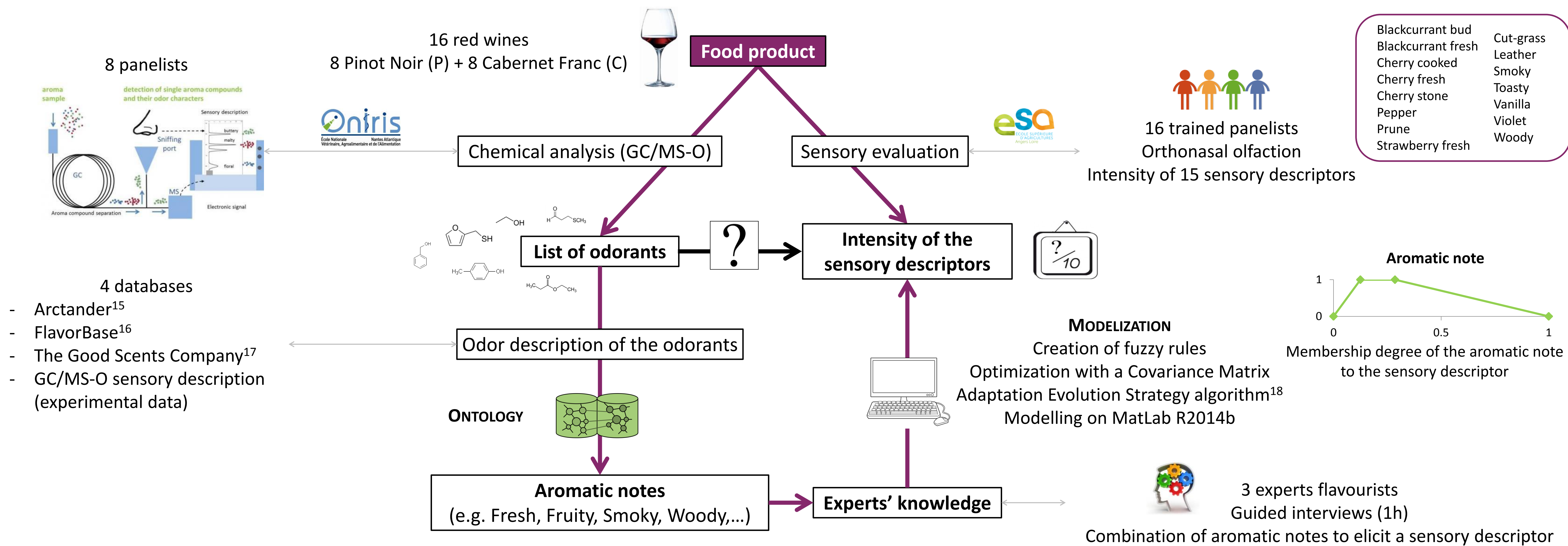
Predictive approaches are now developing to predict the odor characteristics of molecules: detection thresholds^{5,6}, odor quality^{7,8}, odor intensity^{9,10,11}, odor pleasantness^{12,13}

However there are few papers focusing on the odor characteristics of mixtures of molecules¹⁴

PROBLEMATIC

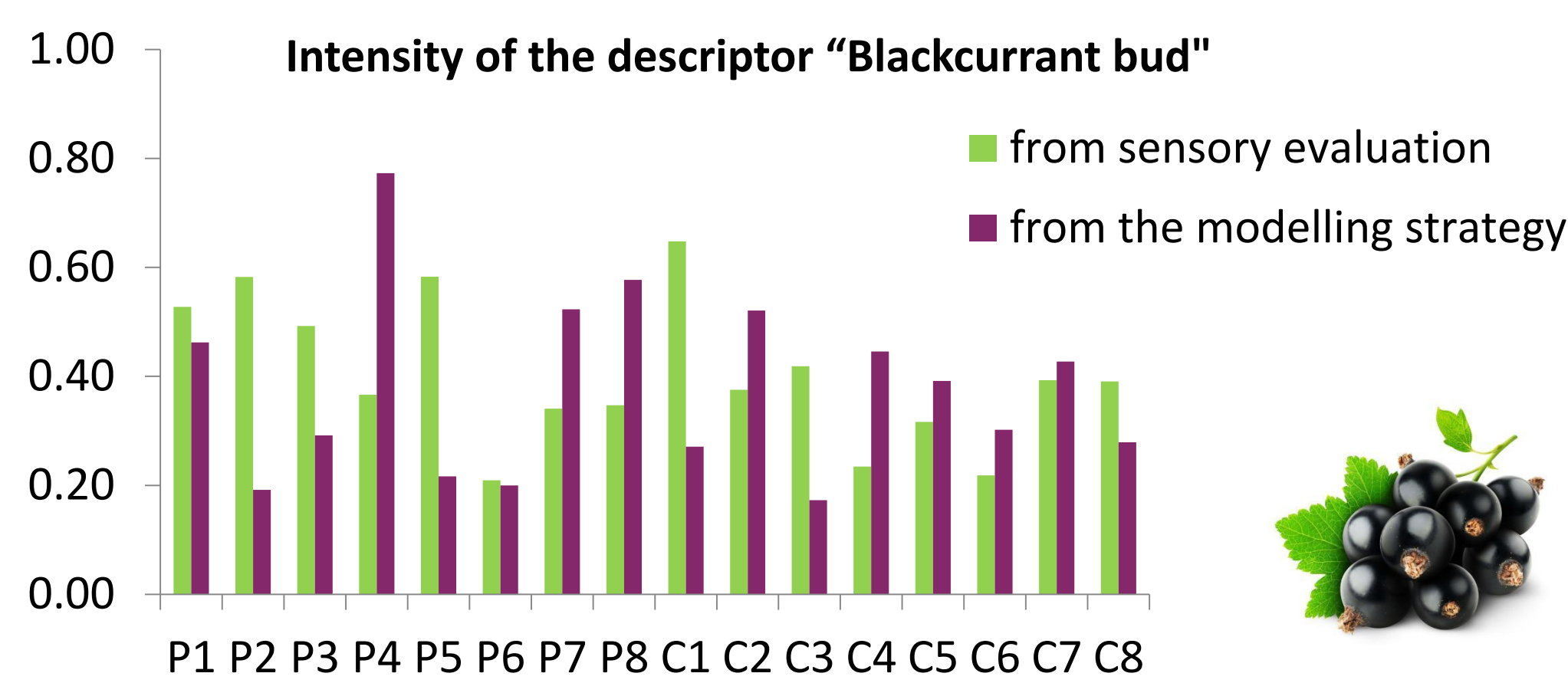
HOW TO PREDICT THE FOOD ODOR PROFILE ON THE BASIS OF ITS COMPLEX CHEMICAL COMPOSITION ?

STRATEGY AND MATERIALS & METHODS



RESULTS & DISCUSSION

Prediction accuracy



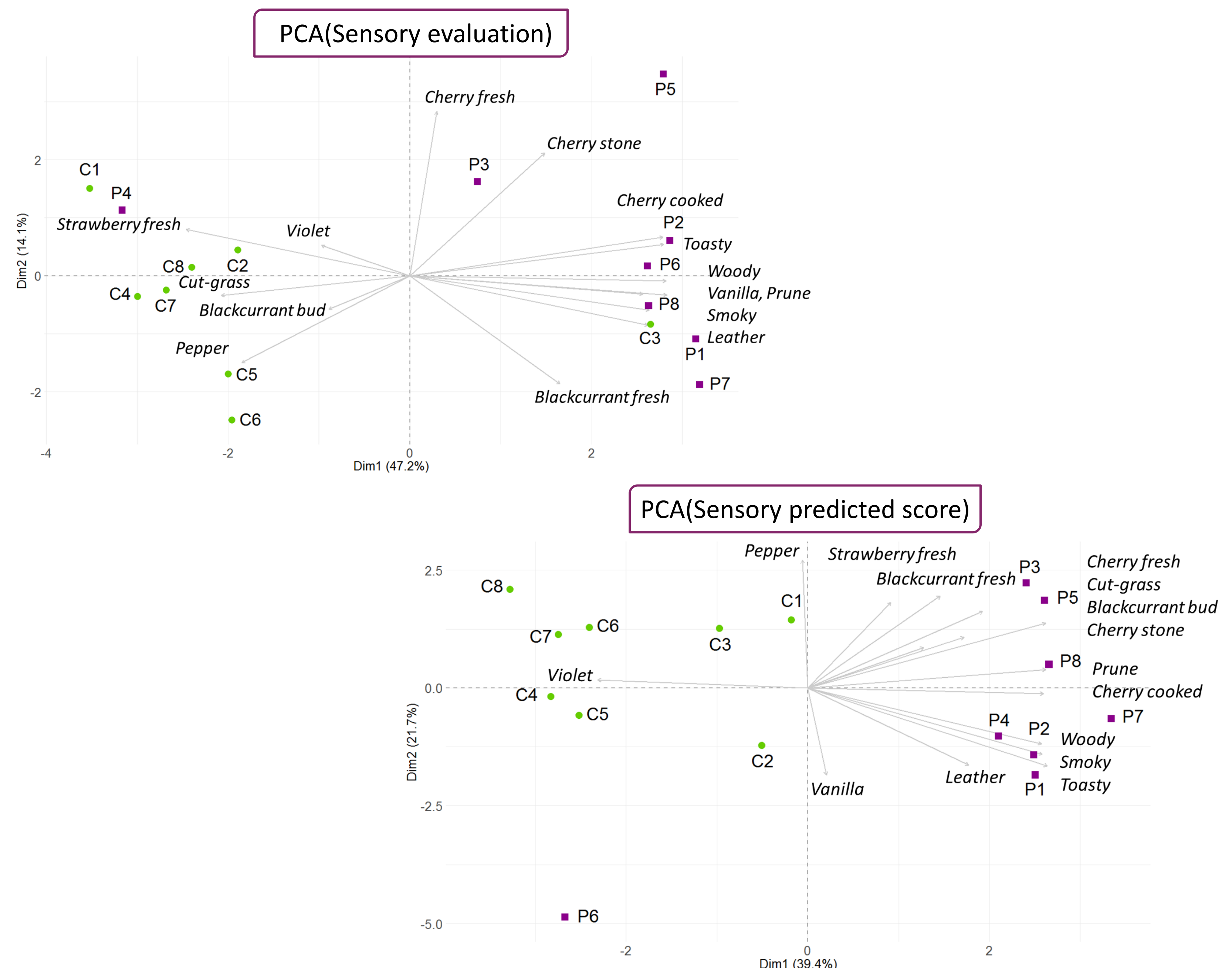
Prediction Accuracy (%)			
P1	99.3	C1	96.2
P2	96.1	C2	98.5
P3	98.0	C3	97.5
P4	95.9	C4	97.9
P5	96.3	C5	99.2
P6	99.9	C6	99.2
P7	98.2	C7	99.7
P8	97.7	C8	98.9
Average = 98 %			

$$PA (\%) = 1 - \frac{|IS - IP|}{10}$$

PA: Prediction accuracy
IS: intensity evaluated by sensory evaluation
IP: intensity predicted
10: maximal difference between IS and IP

The average of the prediction accuracy for the 15 sensory descriptors is higher than 96 %.
But the wine ranking has to be improved.

Principal Component Analysis: PCA(Sensory evaluation)=PCA(Sensory predicted score) ?



CONCLUSION

Promising results => validation of our modelling strategy

Strengths:

Considering the mixture as a whole rather than as a sum of constituents
Integration of flavorists' expertise along the flavor analytical path

Perspectives: databases aggregation, optimization parameters

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