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EXPLORING THE ODORANT AND MOLECULAR CHARACTERISTICS OF MOLECULES SHARING THE ODOR NOTES OF AN AROMA BLENDING MIXTURE



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Scientific Context

Buck & Axel
Cell 1991

The first step of odor perception is an interaction between odorants and olfactory receptors

- odors perceived in our environment are mainly the result of mixtures of odorants
- the specific mechanisms involved in their processing remain poorly understood

Thomas-Danguin et al.
Front. Psychol. 2014

Wilttrout et al.
Behav. Neurosci. 2003

A mixture of odorants **A** and **B** carrying different odors is an odor blending if it is perceived to have a specific new odor, distinct from odors of each component of the mixture **AB** (configural perception)

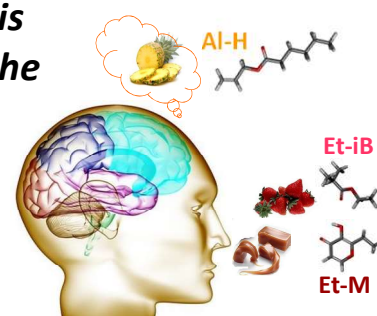
⇒ a blending mixture percept can be represented as: **AB** ≠ **A+B**

Previous studies performed at INRA-CSGA

- A mixture of ethyl isobutyrate (**Et-iB**, strawberry-like odor, **STR**) **A** and ethyl maltol (**Et-M**, caramel-like odor, **CAR**) **B**

was investigated in comparison with a reference (allyl hexanoate, **Al-H**, pineapple-like odor, **PNA**) **C**

the mixture **A+B** was judged as more typical of a pineapple odor than the individual components **A** and **B**



Le Berre et al.
Chem. Senses 2008

Aim of the Study

Exploring the key features of the odors of the aroma blending mixture of **Et-iB** and **Et-M**

- focus on odors, in line with some studies that highlight the significance of this biological function of odorants
- approach based on our recent work related to the analysis of a large odorants database

Ma et al. Proc. Natl. Acad. Sci. U. S. A. 2012
Poivet et al. Sci. Adv. 2018

Odorants descriptions:
Flavor-Base 9th Ed. (2013). Leffingwell & Associates

Tromelin et al. Flavour Frag. J. 2018

We developed an *in silico* approach based on molecules having at least one of the odors **STR**, **CAR** or **PNA**

⇒ dataset of 293 molecules and their related odors was built

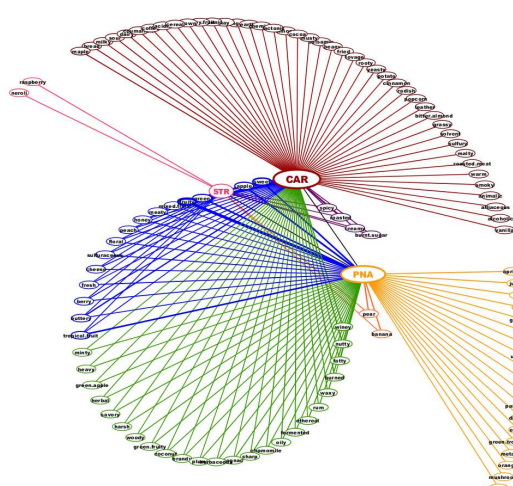
We explore the dataset by two ways:

- the network of the odors using the “social network” notion
- the structural properties of odorants using a pharmacophore approach

Network of odor notes STR, CAR, PNA

Links L1 and L2 between **STR**, **CAR** and **PNA** and to all other odors of the network

172 pairs of odors



Cytoscape Software:
Shannon et al. Genome Res. 2003, 13, 2498

odors links at Level L1:

- 9 links L1 **STR-CAR**
- 4 links L1 **STR-PNA**
- 1 link L1 **CAR-PNA**

odors bridges at Level L2:

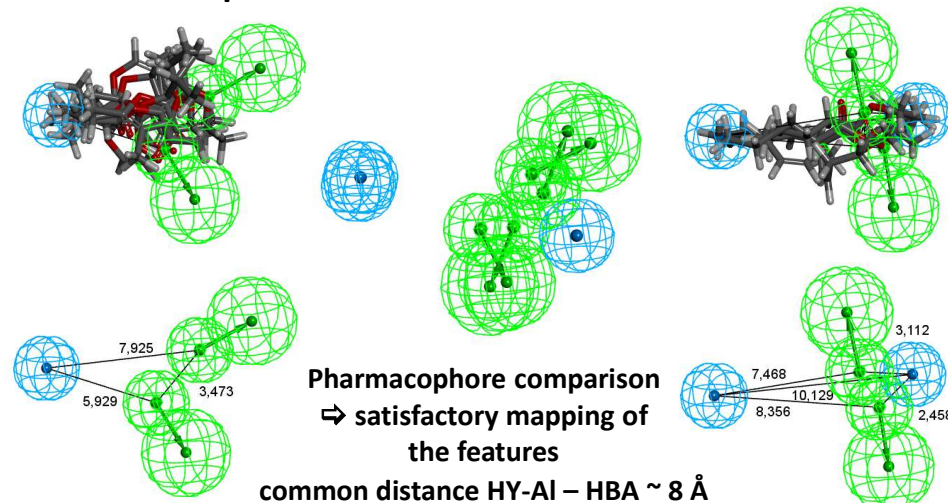
- 15 odors link **STR-CAR-PNA**
- 4 odors link **STR-CAR**
- 2 odors link **STR-PNA**
- 24 odors link **CAR-PNA**

no-bridge odors:

- 2 to **STR**
- 43 to **CAR**
- 19 to **PNA**

Pharmacophores of odorants

Pharmacophore models of 9 **STR-CAR** and 4 **STR-PNA**



STR-CAR: 1 **HY-AI**, 2 **HBA**

STR-PNA: 2 **HY-AI**, 1 **HBA**

Hydrophobic Aliphatic
HY-AI

Hydrogen Bond Acceptor
HBA

Conclusion: The obtained results are in accordance with the hypothesis whereby molecules sharing the odors involved in a blending mixture could recognize a common set of ORs



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