Exploring the odorant and molecular characteristics of molecules sharing the odour notes of an aroma blending mixture

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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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MULTIMIX

Scientific Context

Buck & Axel Cell 1991

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

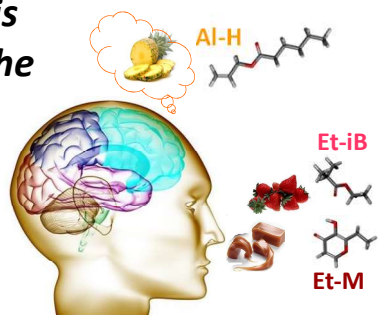
- **odors perceived in our environment are mainly the result of mixtures of odorants**
- **the specific mechanisms involved in their processing remain poorly understood**

Thomas-Danguin et al. Front. Psychol. 2014

Wiltrout 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



Le Berre et al. Chem. Senses 2008

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

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

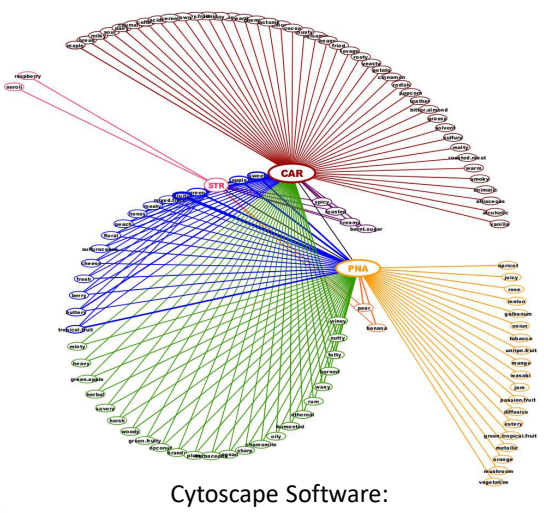
We developed an *in silico* approach based on molecules having at least one of the odors STR, CAR or PNA
⇨ dataset of 293 molecules and their related odors was built
We explore the dataset by two ways:

- **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:

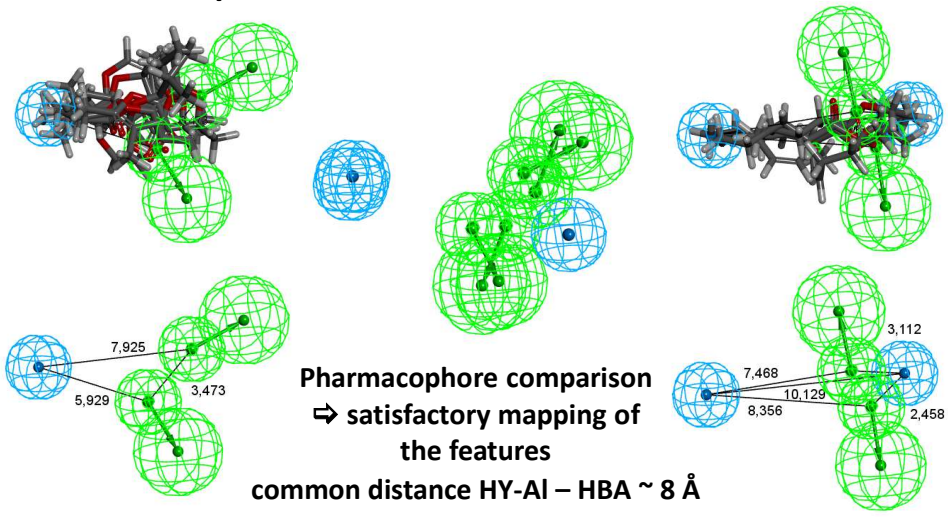
- 15 odors link ST-CAR-PNA
- 4 odors link STR-CAR
- 2 odors link STR-PNA
- 24 odors link CAR-PNA

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



Pharmacophore comparison
⇨ satisfactory mapping of the features
common distance HY-Al – HBA ~ 8 Å

STR-CAR: 1 HY-Al, 2 HBA

STR-PNA: 2 HY-Al, 1 HBA

Hydrophobic Aliphatic
HY-Al

Hydrogen Bond Acceptor
HBA

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

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