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

Anne Tromelin, Florian Koensgen, Karine Audouze, Thierry Thomas-Danguin, Elisabeth Guichard

▶ **To cite this version:**

Anne Tromelin, Florian Koensgen, Karine Audouze, Thierry Thomas-Danguin, Elisabeth Guichard. Exploring the odorant and molecular characteristics of molecules sharing the odour notes of an aroma blending mixture. The 16. Weurman Flavour Research Symposium, May 2021, Virtual meeting (Dijon), France. , 10.5281/zenodo.5948755 . hal-03253812

HAL Id: hal-03253812
https://hal.inrae.fr/hal-03253812

Submitted on 8 Jun 2021

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

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

ANNE TROMELIN[1], Florian Koensgen[1], Karine Audouze[2], Elisabeth Guichard[1], Thierry Thomas-Danguin[1]

[1]Centre des Sciences du Goût et de l'Alimentation, AgroSup Dijon, CNRS, INRAE, Université Bourgogne Franche-Comté, F-21000 Dijon, France;
[2]Université de Paris INSERM UMR-S1124, F-75006 Paris, France

anne.tromelin@inrae.fr

ANR-18-CE21-0006
MULTIMIX

Scientific Context

Buck & Axel Cell 1991

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

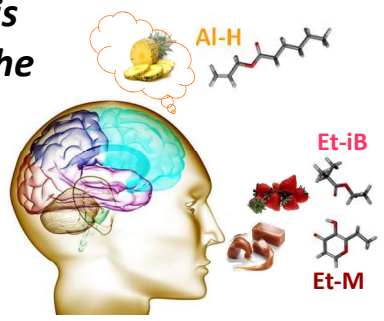
- **odors perceived in our environment are mainly the result of mixtures of odorants**
- **the specific mechanisms involved in their processing remain poorly understood**

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

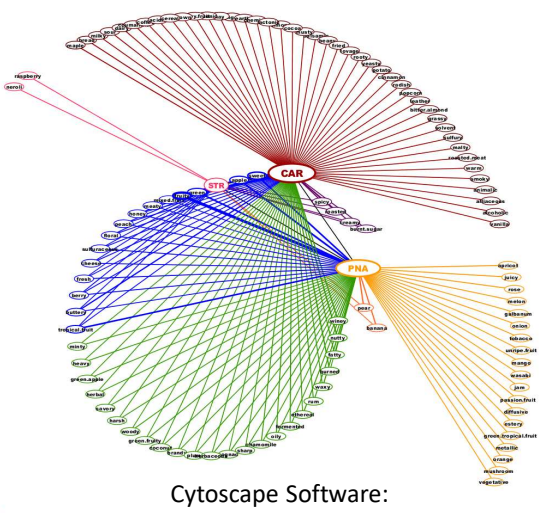
We developed an *in silico* approach based on molecules having at least one of the odors STR, CAR or PNA
⇨ dataset of 293 molecules and their related odors was built
We explore the dataset by two ways:

- **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:

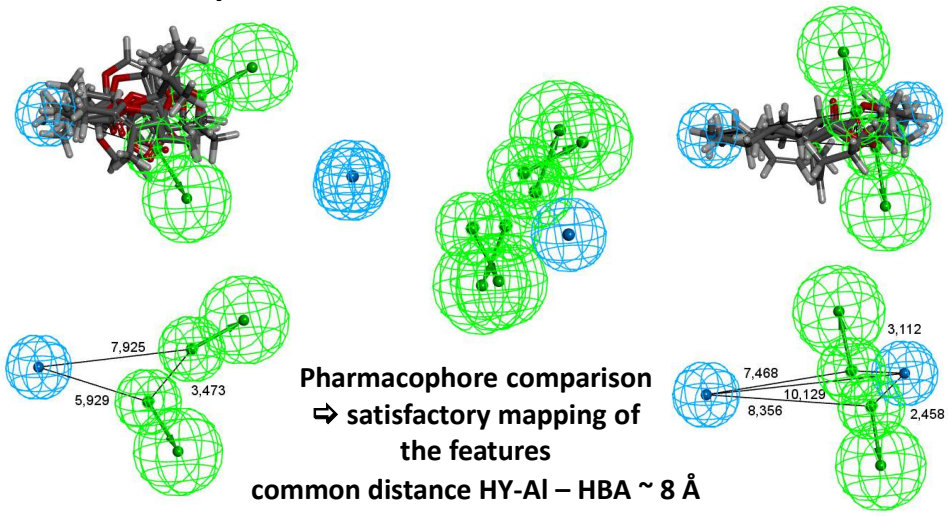
- 15 odors link ST-CAR-PNA
- 4 odors link STR-CAR
- 2 odors link STR-PNA
- 24 odors link CAR-PNA

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

Centre des Sciences du Goût et de l'Alimentation

XVI Weurman Flavour Research Symposium
ONLINE: Live and On-demand May 4-6, 2021
Weurman Dijon 2020