Chemo-biological analysis applied to the olfaction field

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Abstract

Human are surrounded by numerous molecules in the air from a limited number of olfactory receptors, and one odor is not caused by only one compound but by a mixture of molecules[1,2]. Two different perceptions exist, the first being the heterogeneous perception which is the distinction between the odor components of the mixture. The second perception is homogeneous and consists in a mixture of molecules resulting in a single odor which is not possible to distinguish between odor components of the mixture. There are two types of homogeneous perceptions:

1- When one of the mixture components covers the other constituents and we can only smell the odor of one of the mixture components: it is overshadowing or masking.

2- When the perceived/detected odor is different from each of the mixture components: it's an aroma blending mixture or aromatic accord.

In the presented work, we focused on one aromatic accord, which is a simple mixture of two molecules: ethyl isobutyrate (strawberry odor) and ethyl maltol (caramel odor). The mixture of these two molecules is perceived with a pineapple odor (similar to that of allyl hexanoate)[3].

We developed Quantitative Structure Activity Relationships (QSAR) models based of odors of molecules to study the structural characteristics of both caramel (in the mixture) and pineapple molecules as a preliminary study of the aromatic accord they belong to[4]. We extracted the important physio-chemical and structural descriptors of those two odors and find what chemical structure properties describe caramel and pineapple molecules. The final aim being to create the best predictive models.

This study will help to understand the aromatic accord and its mechanism. This also gives an advanced comprehension of the first step of the olfactory system, which leads to more information on the activation of the olfactory receptors (ORs). In a long-term perspective, it will be interesting to use those prediction models to determine if any small molecule has an odor or to know each characteristic of every specific odorant.

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1. Buck L, Axel R. Cell, 1991, 65, 175-187.
2. Thomas-Danguin T, Sinding C, et al. Front. Psychol., 2014, 5, 504.
3. Le Berre E, Thomas-Danguin T, et al. Chem. Senses, 2008, 33, 193-199.
4. Poivet E, Tahirova N, et al. Sci. Adv., 2018, 4, eaao6086.