[P33] *In silico* study of correspondences between odors descriptions linked to common features of aromas compounds

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The first step of odor detection and discrimination of structurally diverse odorants depends of their interactions with olfactory receptors (ORs) [1], whereas the perception of odors quality results from a combinatorial coding [2], whose identification still remains a major challenge. Recently, Martinez-Mayorga *et al*. demonstrated that odor description can be successfully analyzed using a metric approach by performing a descriptive analysis of the Flavor Base database (http://www.leffingwell.com, version 2010) [3].

The current version Flavor Base (9th edition, 2013) is one of the largest collections of flavor molecules (4226 molecules). We extracted 3508 molecules for which the described odors result from an orthonasal perception and identified 251 odor descriptors present in at least 5 molecules. The 3508 odorant molecules and the 251 descriptors have been used to create a matrix whose each element was converted into binary values: 1 when the descriptor appears in odor description, 0 otherwise [3]. We performed an *in silico* study involving correspondence analysis of odor descriptors and hierarchical clustering, showing the existence of several odor groups.

We focused on three odor descriptors associated in several descriptions: “strawberry”, “caramellic” and “pineapple”. Indeed, previous investigations on the perception of a mixture including specific proportions of ethyl isobutyrate (strawberry-like odor) and ethylmaltol (caramel-like odor) have revealed that this specific mixture was especially judged as more typical of a pineapple odor than the individual components [4-8]. Assuming that molecules sharing a same odorant quality possess common structural molecular property [9]), our assumption was that molecule sharing strawberry, caramel or pineapple odor should also share several common structural characteristics. To test this hypothesis, we used Common Feature Pharmacophore Generation protocol (HipHop) implemented in Discovery Studio 2.1 (Accelrys Inc.) [10] to generate pharmacophore hypotheses. We selected 7 molecules described as “strawberry”, 6 molecules as “caramel” and 6 molecules as “pineapple” and then performed HipHop Pharmacophore Generation on each subset separately. A pharmacophore comparison leads to obtain a good mapping of these three pharmacophore models, putting forward a common spatial arrangement of chemical features.

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