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Understanding the odour network

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We live in a sea of data which we interact, inadvertently or advertently, through our senses. Among major sensory modalities, the physical stimulus attributes to perception mapping is more or less well defined in vision and audition, but not in olfaction. Although, the molecular concentration to perceived odor intensity mapping has been established [1], there is no known general systematic relationship of molecular properties onto the olfactory percept. In other words, it has been a challenge to predict the smell of a novel molecule by its physicochemical structure, or the physicochemical structure of a novel smell. There has been a large progress in this decade towards understanding the molecular and neural basis of olfactory perception [2], [3], [4], [5], [6], [7]. Khan *et. al* predicted the odor pleasantness based on odorant structure and they considered odorant database of 144 odorants [8]. Kermen *et. al* [9] reported the relationship between olfactory note and molecular structure recently. The knowledge of chemistry, odor scientists and efforts of IBM [10] has given us huge database of almost 31 million molecules along with their physical, structural and other properties. This dataset is not structured in terms of odor, and no attempt has been made to understand and organize this huge data in olfaction space. One of the most important aspects of understanding the data is visualization. Recently, network analysis has grabbed much attention due to its clear representation in terms of entities and relationship and more often than not, they provide some really interesting insights into the data they represent [11]. The present work aims at discovering inherent statistical structure in large chemical and perceptual databases available online in order to derive principles for predicting odor perception from the chemical structure of odorants via network analysis of Flavournet dataset. The Flavournet dataset consists of 738 odorants arranged by chromatographic and sensory properties. An adjacency list of odorants on the basis of perceived smell was created. Further, an ***odor network*** was created in which each odorant forms the node and weight of edge between them shows the number of odors they share with each other. The initial results give very good insights about the dataset such as there are two islands in this network. The fully connected smaller island is only inhabited by alkane family of odors and the bigger island follows the degree distribution of a scale free network. Further, the physical and structural descriptors were superimposed on this graph in order to understand it in a better way. The results provide useful insights into the odor space.

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