

## Odor Clustering Based on Molecular Parameter for Odor Sensing

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Odor sensors can benefit various areas of human activity and have been increasingly studied. For developing odor sensors, comprehensive detection of numerous volatile molecules is necessary. These advanced odor measurements might be accomplished by inspiring technology based on the bio-olfactory system. This system recognizes and discriminates odors by activity patterns, which are formed based on odor information of odorants extracted from olfactory receptors (ORs). Hence, odorants are appropriately categorized into clusters with different molecular features. The odor clustering close to biological olfaction can also be applied to the sensor systems. In this study, odor map images of rats investigated in biological studies were analyzed by principal component analysis (PCA) to clarify odor clustering features of olfaction. The definition of odor cluster and extraction of geometric features of odor maps were examined based on the primary components and factor loadings. Then, key parameters expressing clusters and measurable in sensor technology were successfully explored by evaluating the correlation between principal components and molecular parameters calculated using the molecular modeling software. Finally, artificial odor maps were reconstructed based on the defined odor clustering map, and the similarity between odor maps of rats was confirmed.

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