

# STATISTICAL CLUSTERING OF ODORANT MOLECULES BASED ON BOTH MOLECULAR PROFILE FEATURE EXTRACTION AND OLFACTORY BULB ODOR MAP IMAGING ANALYSIS

Liang SHANG, Chuanjun LIU, Kenshi HAYASHI

Kyushu University

shang.liang.100@s.kyushu-u.ac.jp

It is significant to study the relationship of olfactory bulb response patterns (olfactory images) to odorant molecule features for understanding the mechanisms of mammalian olfactory. In this study, 178 odorant olfactory images (OI) in rat olfactory bulbs and 49 varieties of molecular parameters (MP) had been analyzed to explore the relationship between odorants' molecule parameters and their olfactory images. Firstly, correlation coefficient between the grey-levels on pixels of olfactory images and parameters of odorants were calculated. Correlation coefficient maps for molecule parameters were established. Hierarchical clustering analysis was performed for correlation coefficient maps. The cluster results showed that all parameters were divided for 7 clusters, and a relatively similar response pattern was found in each cluster. T-distributed stochastic neighbor embedding (t-SNE) was employed for mapping odorants in 2D spaces by olfactory images and molecular parameters (Fig. 1), respectively. It suggests that some odorants are similar in molecular space, but they would be different in olfactory space. Finally, based on the features extracted by PCA or t-SNE from OI and MP, functional group identification models were calibrated by artificial neural network (ANN), include learning vector quantization (LVQ), support vector machine (SVM) and extreme learning machine (ELM), respectively. The model calibrated by ELM based on OI-PCA, whose accuracies for calibration and validation set reached 94.81 % and 93.02 %, respectively, had a good potential in identifying function groups for 178 odorants. The results indicated that olfactory images contained more information than 49 molecular parameters.

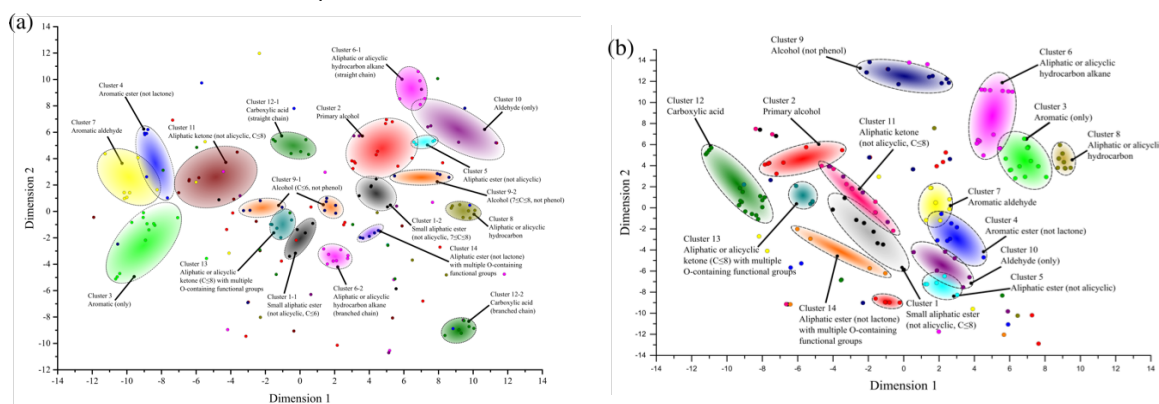


Fig.1. Artificial maps generated by olfactory images (a) and molecular parameters (b) for 178 odorants from 14 types of functional groups by t-SNE method. Each point indicates an odorant.