# Development of Olfaction Inspired Odor Sensor Based on Structure-odor Relationships

商, 亮



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氏　　名　：商　亮

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（匂いと分子構造の関係に基づく嗅覚模倣匂いセンサの開発）

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# 論　文　内　容　の　要　旨


As the most primitive sense, olfaction plays an essential role in our daily lives, which provides us an opportunity to explore our chemical environment. Progress in the molecular biology of olfaction has revealed a close relationship between the structural features of odorants and the response patterns they elicit in the olfactory bulb. Molecular feature-related response patterns, termed odor maps (OMs), may represent information related to basic odor quality. To understand the structure-odor relationship is very helpful for clarifying the mechanism of bio-olfaction and developing olfaction-inspired odor sensors. Accordingly, this research aims for exploring the relationship between olfaction information and molecularly information of odorants, and developing a molecular recognized optical sensor platform for volatile organic compounds (VOC) detection and identification. This dissertation consists of seven chapters and the chapter outlines are described as follows:

Chapter 1 composed the background of the present study. The general introductions on the mechanism of bio-olfaction model and odor sensors were reviewed. Also, the basic characteristics and mechanism of localized surface plasmon resonance (LSPR) and molecularly imprinted sol-gels (MISGs) were presented.

Chapter 2 explored the correlation between OMs and the molecular parameters (MPs) of odorants by taking OMs from rat olfactory bulbs and extracting feature profiles of the corresponding odorant molecules. Correlation analysis between the two matrixes was first carried out by establishing coefficient maps. Results from hierarchical clustering showed that all parameters could be segregated into seven clusters, and each cluster showed a relatively similar response pattern in the olfactory bulb. Using the information from the OMs and MPs, we mapped odorants in 2D space by incorporating dimension-reducing techniques based on principal component analysis (PCA) and t-distributed stochastic neighbor embedding (t-SNE). Artificial neural network models based on the OM and MP feature values were proposed as a means to identify odorant functional groups. An OM-PCA-based model calibrated via extreme learning machine (ELM) was 94.81% and 93.02% accuracy for the calibration and validation sets, respectively. Similarly, an MP-t-SNE-based model calibrated by ELM was 86.67% and 93.35% accuracy for the calibration set and the validation set, respectively. This research supports a structure-odor relationship from a data-analysis perspective.

Chapter 3 presented a proof-of-concept model by which odor information can be obtained by

machine-learning-based prediction from MPs of odorant molecules. The features of the MPs were extracted via either unsupervised or supervised approaches and then used as input to calibrate machine-learning models. Predictions were performed by various machine-learning approaches. A support vector machine model combined with feature extraction by Boruta (confirmed only) was found to afford the best results with an accuracy of 97.08%. The result indicated that ODs can be predicted by machine-learning-based models from MPs.

Chapter 4 explored a possibility to use LSPR of Au nanoparticles (AuNPs) and MISGs as the sensitive layer to recognize typical organic acid odorants. The LSPR layer was prepared by vacuum sputtering of AuNPs on a glass substrate and consequently thermal annealing. The sensitive layer was fabricated by spin-coating molecularly imprinted titanate sol-gel on the AuNPs layer. For the MISG coated sensors, the LSPR sensitivity was affected by the spin coating speed. In addition, a sensor array based on MISGs with different templates was constructed to detect the organic acids in single and their binary mixtures. A 100% classification rate was achieved by leave-one-out cross-validation technique for linear discriminant analysis model. It demonstrated that the MISGs coated LSPR sensor array has a great potential in organic acid odor recognition of human body odor.

Chapter 5 developed a sensitive and selective nanocomposite-imprinted, LSPR sensor for cis-jasmone vapor. The functional monomer and the ratio of matrix materials to functional monomers in the MISGs were investigated and optimized. MISGs that contained the functional monomer trimethoxyphenylsilane at a 3:1(v:v) ratio exhibited a higher sensitivity and selectivity than other films.

In Chapter 6, AuNPs were doped in the MISG to enhance the sensitivity of the LSPR sensor through hot spot generation. The size and amount of AuNPs added to the MISG were investigated and optimized. The sensor coated with the MISG containing 20 μL of 30-nm AuNPs exhibited higher sensitivity than that of the sensors coated with other films. Furthermore, an optical multi-channel sensor platform containing different channels that were bare and coated with four types of MISGs was developed to detect plant VOCs in single and binary mixtures. k-nearest neighbor model had good potential to identify plant VOCs quickly and efficiently (96.03%). This study demonstrated that an LSPR sensor array coated with an AuNP-embedded MISG combined with a pattern recognition approach can be used for plant VOCs detection and identification.

Chapter 7 summarized the experimental works and concludes the dissertation with recommendations for future work.