

論文 / 著書情報  
Article / Book Information

題目(和文)	
Title(English)	Machine learning for Scent: Forward and Inverse Perceptual model for Olfactory perception using mass spectrum of Odorant Molecules
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学位種別(和文)	博士論文
Category(English)	Doctoral Thesis
種別(和文)	論文要旨
Type(English)	Summary

(博士課程)

Doctoral Program

## 論文要旨

THESIS SUMMARY

系・コース  
ス：  
Department of, Graduate major in

Information &  
Communications  
Engineering

系  
コース

申請学位（専攻分野）：  
Academic Degree Requested  
博士  
Doctor of  
(Engineering)

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要旨（英文 800 語程度）

Thesis Summary (approx.800 English Words)

Olfactory perception of a flavor molecule is an important research topic in machine olfaction domain which is necessary for controlling the sensory attributes of the final product with a scent. Previously physicochemical properties, sensor data, molecular fingerprint were used as an input for modeling the odor impression task. But we cannot use such olfactory stimuli or sensing data for chemical mixtures since natural odor in our daily life is a mixture. Out of other olfactory stimuli we use mass spectrum dataset as an input and binary odor descriptor (peach, sweet etc.) as output to build an odor prediction model. Our target is to create scent by blending different components of odorant molecules. So, at first, we establish a method to predict the odor impression from the imbalanced dataset because more than half of the descriptors rarely appear. None of the works reported the solution of imbalanced problem in machine olfaction (odor impression prediction) in terms of using original dataset. This problem occurs quite often since only a few descriptors frequently appears in most of cases. We successfully predict 89 odor descriptors from the Leffingwell database using one class support vector machine as only negative samples are enough for training the model. We found a statistically significant prediction performance compared to graph neural network models (using the same dataset) for small category odor descriptors.

After successfully predicting individual odor descriptors, our next goal is the inverse model, that means, the prediction of the sensing data for a given binary odor descriptors. Although previous work predicted the mass spectrum for an odor descriptor based on continuous sensory information, it cannot handle the binary sensory information such as 'peach', 'vanilla'. It is difficult to predict odorant's sensing data associated with binary odor descriptors because we need to find the sensing data similarity based on an intended scent impression. We used Self Organizing Map to cluster chemical compounds into a group for a binary odor descriptor to label them based on their mass spectra, which is closely related to their chemical structures. Chemical compounds with similar mass spectra trigger similar olfaction sensations. These findings are supported by sensory evaluation. This study is the first report for predicting sensing data for a given binary scent impression.

Previous works tried to solve the problem of perception of odor mixture. But in the term of sensing data, it has not been solved yet. Since there is no dedicated software to calculate the structural properties of the odorant mixture, it hinders the progress of the perception of the odor mixture. However, the mass spectrum is a good way for predicting odor mixtures because it can be used for both mono-molecules and chemical mixtures and linear superposition is valid in mass spectrum. We used the binary mass spectrum mixture of two different group essential oils to predict the scent impression. As this is the first time, we reported the mixture odor prediction using mass spectrum, we only predicted the sweet odor impression. The sensory test revealed that the prediction of binary mixture of the essential oils was almost successfully achieved. It can be extended to other descriptors also. Although our work on chemical mixtures in initial stage, we hope that future works will be done based on this work to establish the real-world chemical mixture perception.

備考：論文要旨は、和文 2000 字と英文 300 語を 1 部ずつ提出するか、もしくは英文 800 語を 1 部提出してください。

Note : Thesis Summary should be submitted in either a copy of 2000 Japanese Characters and 300 Words (English) or 1copy of 800 Words (English).