Q-AOS 九州大学 アジア・オセアニア研究教育機構 ブラウンバッグセミナー

Brown Bag Seminar No.190

2025 6.11 (wed.) 12:10 ~ 12:50

12:10-12:15 ◆ Introduction
12:15-12:40 ◆ Seminar (Presentation)
12:40-12:50 ◆ Q&A

Online (Zoom)
Scan here for Registration

https://us02web.zoom.us/webinar/register/WN_CR46OfdKTB6sbNVNAXgdNA

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Machine Learning for Predicting Odor Characteristics from Molecular Structures

3 GOOD HEALTH AND WELL-BEING
9 INDUSTRY, INNOVATION AND INFRASTRUCTURE

Key Words

Odor

Cheminformatics

Artificial Intelligence

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After working at Tohoku Univ., Tottori Univ. and RIKEN (Drug Discovery Computational Chemistry Platform Unit and Advisory Council On Cluster for Science, Technology and Innovation Hub), I assumed my current position.

I am interested in the informatization of odor since my doctoral period. I proceed the current research by leveraging the background in chemistry and information science, along with understanding of flavor and fragrance creation.

The relationship between the molecular structure and psycho-biology of odors remains still unclear. Recently, we reported a regression analysis based on odorant chemical space. We discussed the prediction performance (predictability of odor descriptor) depends on "structural diversity" for the groups associated with each odor descriptor. The strong influence is traced between structural diversity and the predictability of odor descriptor. We carried out the analysis by four molecular fingerprints, the essential arguments are qualitatively conserved among them. In this investigation, we encountered difficulties related to the complexity included in the odor descriptor. We believe that this study broadly proceeds odor prediction and paves the way toward digitizing odors.