

# Food digital transformation: large-scale prediction of food functions and elucidation of the mode-of-action

**Tomokazu Shibata**<sup>1</sup>  
shiba535@bio.kyutech.ac.jp

**Yusuke Tanaka**<sup>2</sup>  
yusuke-tanaka@housefoods.co.jp

**Hiromu Taguchi**<sup>2</sup>  
h-taguchi@housefoods.co.jp

**Ryusuke Sawada**<sup>1</sup>  
sawad330@bio.kyutech.ac.jp

**Morihiro Aoyagi**<sup>2</sup>  
m-aoyagi@housefoods.co.jp

**Takashi Hirao**<sup>2</sup>  
t-hirao@housefoods.co.jp

**Yoshihiro Yamanishi**<sup>1</sup>  
yamani@bio.kyutech.ac.jp

<sup>1</sup> Department of Bioscience and Bioinformatics, Kyushu Institute of Technology,  
680-4 Kawazu, Iizuka, Fukuoka 820-8502, Japan

<sup>2</sup> Research and Development Headquarters, House Foods Group Inc.,  
1-4 Takanodai, Yotsukaido, Chiba 284-0033, Japan

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The aging of the population in developed countries, including Japan, has led to the problem of increasing medical costs. It is important to extend healthy life expectancy so that people can lead healthy and cultured lives. Daily food intake is closely related to health, and it would be ideal if we could maintain health through our daily diet. Since foods contain a wide variety of constituent compounds, there is a high possibility that they have unknown food functions and health effects. Even if food functions are known, it is very difficult to understand the mode-of-action.

In this study, we developed a machine learning method to comprehensively predict food functions and the mode-of-action based on a vast amount of food-related data. In contrast to our previous study on the prediction of health effects of food peptides [1], the scope of this study is not limited to peptides but covers all possible constituent compounds of foods. First, we collected information on the chemical structures of 69,594 constituent compounds for 757 foods from literature and databases. Next, using 1,830,624 compound-protein interaction pairs (1,288,343 compounds and 4,643 proteins) as training data, we constructed machine learning models to predict compound-protein interactions, and comprehensively predicted the proteins with which food constituent compounds interact. To estimate food functions, we linked the food constituent compounds to applicable diseases based on known therapeutic targets of 649 diseases. The correspondence between the therapeutic target proteins and the applicable diseases was manually collected from literature data. Finally, we predicted a large-scale network consisting of four types of nodes (foods, constituent compounds, target proteins, and applicable diseases), and elucidated the mode-of-action of the predicted food functions. For each food, the functional associations among target proteins were also examined at the pathway level. The proposed method is expected to be useful not only for prediction of food functions but also for elucidation of the mode-of-action.

[1] Fukunaga, I.; Sawada, R.; Shibata, T.; Kaitoh, K.; Sakai, Y.; Yamanishi, Y. Prediction of the Health Effects of Food Peptides and Elucidation of the Mode-of-action Using Multi-task Graph Convolutional Neural Network. *Molecular informatics*, 2020, 39, 1900134.