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# Predicting optimal natural compounds that modulate multi-targets for type 2 diabetes mellitus-related complications

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Various natural compounds have great potential to be used as functional materials or candidate materials for new drugs, so it is very important to discover substances with excellent biological activity. However, discovering bioactive substances using traditional methods is time-consuming and expensive. There were limitations in selecting optimal compounds from a very large pool of candidates. Therefore, various machine learning models have recently been developed to discover promising natural products, but they have limitations in that they are limited to predicting a single target protein or are unable to predict target proteins with insufficient protein-compound interaction data. To solve this problem, this study developed prediction model using Siamese Neural Network (SNN) for a multi-target protein regulating natural compound. This model has a structure that includes a multi-layer neural network for deep learning, internalizing the functions of end-to-end learning and variable selection, and can learn multi-label data to predict the activity of natural compounds against multiple target proteins. In addition, it is meaningful in that it is a model that can be applied to target proteins with insufficient data by designing it to perform few-shot learning. To examine the applicability of this model, natural compounds that regulate multiple target proteins related to type 2 diabetes complications and food materials containing them were discovered. Among them, it was confirmed that ginger contains the most advantageous natural compounds composition, and the reliability of the model was confirmed by verifying through previous literature that candidate compounds derived from ginger actually have an effect in regulating signal transductions of complications of type 2 diabetes.