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Making sense of large amounts of data is helping NAIST researchers understand metabolites.

Metabolomics

Matching structure to function

A systems biology approach pairs hundreds of structurally distinct metabolite groups to their corresponding functions

Organisms — from bacteria and plants to humans — generate a diverse array of chemicals called metabolites, which play many important roles, such as inducing growth, serving as antimicrobial agents and fighting the growth of tumours.

"The result could aid in the identification of the functions of newly discovered metabolites and the design of new drugs."

Now a team of researchers, including Shigehiko Kanaya from NAIST, have used databases they have developed that classify the chemical structure and biological function of thousands of metabolites across many species, to group metabolites with similar structures into those with similar functions[1]. The result could aid in the identification of the functions of newly discovered metabolites and the design of new drugs.

Metabolomics — the study of metabolites — is a very complex field. Some metabolites are unique to a particular species, while some are seen across multiple species. Some metabolites have a unique function; some have multiple functions. The extent to which clear themes can be identified in how metabolites function will allow researchers to fashion a better understanding of newly discovered metabolites. Systems biology approaches that aim to make sense of large amounts of data are key drivers in understanding metabolomics.

Kanaya and colleagues therefore took a systems approach to the question of how metabolite structure could provide insights into metabolite function. They began by studying the structure of over two thousand metabolites across many species and grouping together those metabolites that had similar chemical structures.

The team identified 671 structurally distinct groups among the metabolites studied. They then categorised each metabolite according to 140 different biological functions from a metabolite activity database, and looked for relationships between a given chemical structure group and a given biological function. This analysis revealed the existence of 983 structure–function pairings.

Although more than 70% of the structural groups could be clearly linked to one or more biological activities, the remaining structural groups could not be definitively classified in this manner, in part because the metabolites that made up those structural groups had multiple divergent functions.

These analyses will provide a guide for researchers in the field of metabolomics to be able to link a newly identified metabolite for which a structure is known with a biological function, and could aid in the development of new medicines.

Reference

1. Ohtana, Y., Abdullah, A.A., Altaf-Ul-Amin, M., Huang, M., Ono, N. *et al.* Clustering of 3D-structure similarity based network of secondary metabolites reveals their relationships with biological activities. *Molecular Informatics* **33,** 790-801 (2014).

More information about the group's research can be found at the Computational Systems Biology Laboratory webpage:
http://isw3.naist.jp/Contents/Research/ai-06-en.html