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Construction of a computational platform for metabolic pathway design

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Computational design of metabolic pathways has become an essential and complementary approach to identify metabolic pathways for the production of chemical products. In order to find the metabolic pathways of value, it is primarily necessary to utilize comprehensive chemical and enzymatic information to ensure a wide range of the enzymatic reaction, and obtain pathway candidates including putative compounds and enzymatic reactions. We have developed an efficient algorithm and a computational tool for the design of extensive metabolic pathways.

The design tool begins the search for metabolic pathways with the initial and last compounds as queries. In the result viewer, the candidate list of metabolic pathways is presented with ranking scores, and the changes in the chemical structures in the metabolic pathways can be checked at a glance. The putative candidates for reactions and compounds are displayed with scores based on the comparison of structural similarities. The design tool provides a user with various design options including the number of reactions, reaction steps and so on. Any chemical and reaction information can be also applied to the design tool, which will be a powerful tool to identify unknown metabolic pathways of chemical products.