[L1] Novel Method Proposing Chemical Structures with Desirable Profile of Activities Based on Chemical and Protein Spaces

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Active molecules among numerous chemical structures in a chemical database can be easily searched by statistical prediction of compound–protein interactions (CPIs). However, constructing a simple prediction model against one protein does not help drug design, because detecting chemical structures that act similarly against multiple proteins is necessary for preventing side effects of the potential drug. To tackle this problem, we propose a new method that visualizes the chemical and protein spaces.

For simultaneous visualization of both spaces, we employ a counterpropagation neural network (CPNN) and develop a new visualization method named multi-input counter-propagation CPNN (MICPNN). In a case study of the kinase protein family, the MICPNN model accurately predicted the complex relationships between the compounds and proteins. The proposed method identified the chemical structures with promising activity against the kinases. Our proposed method is also applicable to other protein families, such as G-protein coupled receptors, ion channels and transporters.