Dr Kimita Funatsu gave this presentation at the International Symposium on Compound Design Technologies held in Tokyo and Osaka, Japan on 19 and 20 March 2014.

Abstract

On the first stage of development of new drugs, various lead compounds with high activity are required. To design such compounds, we focus on chemical spaces defined by structural descriptors. New compounds close to areas around which highly active compounds exist will show the same degree of activity. Therefore we have been developing a new system of structure generation for searching a target area in chemical spaces. First, highly active compounds are manually selected as initial seeds. Then, those seeds are entered to our generator and structures slightly different from the structures of the seeds are generated and pooled. Next seeds are selected from the new structure pool with the scores based on distance from target on the map. In this study, we used GVK data of ligand-binding affinity to verify the advantage of our generator. Visualization of the chemical space and structure generation were performed, and then the outputs were compared with test data. As a result, our generator could produce many structures similar to the test data, which exist near the target area. This result shows that exploration of the target area on the chemical space was performed.

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