Omics-based chemical structure generation considering molecular properties via deep reinforcement learning

Yuki Matsukiyo
Nagoya University

In drug development, identifying a molecule with the desired bioactivity is important but extremely difficult. The main reason is that the number of theoretically possible compounds exceeds 10^60 and it is infeasible to experimentally test all candidate compounds. In order to address this issue and narrow down the candidate compounds for experimental evaluation, chemical structure generators based on deep generative models such as variational autoencoder have been actively applied to de novo drug design. Moreover, omics-based structure generators generating molecules from gene expression profiles about target proteins have also been developed. These methods enable us to generate molecules with the desired bioactivity, considering comprehensive biological information within the cell. However, most existing omics-based structure generators focused on molecular generation reflecting gene expression profiles and few considered other molecular properties (e.g., quantitative estimate of drug-likeness). In this study, we propose a structure generator using deep reinforcement learning that enables property-optimized omics-based molecular generation. We tried to optimize some properties of molecules generated from gene expression profiles, confirming that the proposed method can generate molecules with superior properties to those generated by the existing omics-based structure generators.