Detouring costly quantum-chemistry calculations: Machine-learning prediction of electronic-sturcture-informatics (ESI) descriptors

Yusuke Aikawa, Kumamoto University

We have proposed an Electronic Structure Informatics descriptor. This descriptor is calculated using quantum chemical calculations. The most important point is that it is composed of values that can logically explain chemical reactions and are observable. We believe that using this descriptor to predict the effects of drugs will make predictions more logical from the viewpoint of chemical reactions. The disadvantage is that it takes an a lot of time to calculate the descriptor. To alleviate this problem, we examined a simple prediction method using the RDKit descriptor, which is a representative open-source chemical descriptor. We also examined whether it is possible to interpret what the predictions are based on and whether the interpretation is likely to be correct. The subject is an α-glucosidase inhibitor.