Locally-Described Electronic-Structure Informatics: An Application to Predict Regioselectivity of Glutathione Adducts to Quinone Derivatives Molecules

Y. Tsutsumi, Kumamoto University

We have been proposing "Electronic-Structure Informatics (ESI)", which focuses on electronic features of molecules. So far, the ESI descriptors describing molecular characteristics, which can be classified as “global descriptors”, have been used in machine learning studies on biological activity of drug molecules. Herein, we report “locally-described electronic structure informatics” in which quantum chemical descriptors defined on individual atoms in a molecule are introduced. It will be shown that the new descriptor set can be successfully applied in deep learning using the graph convolutional neural network (GCN) algorithm for prediction of regioselectivity in glutathione adduct to quinone derivatives. The newly developed method is expected useful to predict metabolic reactions in human body.