Predicting Ligand-Receptor Interaction Energies by Electronic-Structure Informatics

Mio Yokoyama, Kumamoto University

Electronic-structure informatics (ESI) is applied to predict ligand-receptor binding energies using fragment-molecular orbital (FMO) method. The binding energies were obtained by the FMO database (FMODB). The ESI descriptors suggested by Sugimoto et al. are used in machine learning. It will be shown that the predicted binding energies well correlation of the FMODB data, indicating the present method can be applied to in-silico screening of small molecules to be strongly bound to receptor proteins.