

## **Development of fingerprints considering chemical reactions**

Kazufumi Ohkawa, Asahi Kasei Pharma

The process of protein-compound association and dissociation can be regarded as a chemical reaction in which the final state does not change from the initial state, and in particular, the change in electron density before and after the binding state is considered to play an important role in binding. In order to account for this change in electron density, we have developed a fingerprint that takes into account the Fukui function, and we report on this method with examples.