Current in the data-driven synthesis route development methods in TS technology (DSRDM in TST) and its applications for fine chemicals

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We have been researching DSRDM, a data-driven synthetic route development method that combines synthetic route development systems such as TOSP/KOSP with theoretical calculations. The aim of this research is to reduce the time required to develop a synthesis route for a new compound to 1/4 of the time currently consumed using current technology. This is thought to be achievable by conducting synthetic experiments based on the predictions of computational chemistry and information chemistry. As one of the NEDO projects for 2022, a project based on this technology was adopted. Over the three years of this project, significant progress has been achieved in technologies that contribute to the digital transformation (DX) of the chemical industry. In this lecture, we will discuss the following results related to the project

(1) Development of AIst-syn, a new synthetic route design system (SRDS), and some results for target compounds using synthetic routes designed using this system

(2) Classification using the characteristics of transition state motifs for many elementary reactions (about 1000 reactions)

(3) Prediction of activation free energy of pericyclic reactions using the Counter-Propagation method

(4) Analysis of catalytic reactions and analysis of the catalytic reaction database (CATRDB), which collects CASTEP calculation results

(5) Current status of the transition state database (TSDB)