Data-Driven Chemistry for Developing Organic Synthesis Routes for Functional Chemicals.

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We have been developing a synthesis route development method called data-driven chemistry, which combines a synthetic route development system (SRDS) and theoretical calculations. This method performs (1) creating synthetic routes using chemoinformatics and (2) calculate transition state (TS) searches using quantum mechanical calculations. Recent AI synthetic route design systems cannot create synthetic routes beyond teaching data since they create synthesis routes based on big data and their machine learning. On the other hand, AIPHOS/TOSP, which uses "transforms", the knowledge of name reactions, has potential to create synthetic routes that have never been considered before. It is known to be very difficult to locate TS for digital screenings without knowledge of chemical reactions and quantum chemistry. We offered a TS Motif method, that takes into account the similarity among transition states, in order to solve this problem. We are also building a database of TS motifs. The TS motif method using TSDB is made it possible to digitally verify a large number of synthetic routes from SRDS in short time. In this lecture, we will show how to perform the data-driven organic synthetic route development by using actual examples we have done.