【Grant-in-Aid for Transformative Research Areas（A）】

Section II

Title of Project： Digitalization-driven Transformative Organic Synthesis （Digi-TOS）

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Number of Research Area：21A204　Researcher Number：10313123

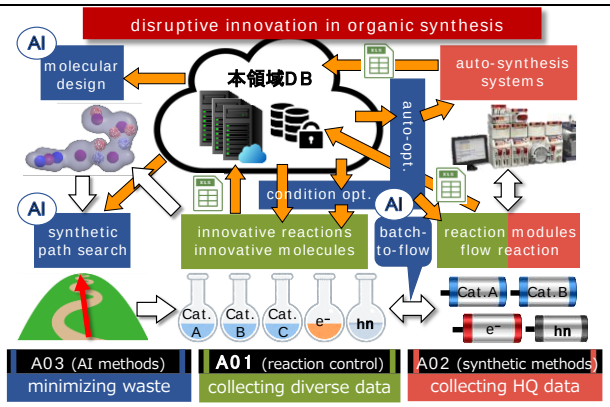
【Purpose of the Research Project】

Synthetic organic chemistry supports manufacturing by creating highly complex and valuable molecules from readily available organic materials. Synthetic organic chemistry currently faces major changes based on digitalization. Artificial intelligence (**AI**) has already made significant achievements in life sciences and materials science. In the field of synthetic organic chemistry, there are also high expectations for AI technology. The use of machine learning (**ML**) for optimizing reaction conditions and searching synthetic routes is being promoted, but the use is still limited because the number of data required for ML is huge, descriptors that capture the essence of the rection are necessary to build a highly accurate ML model, the accuracy of the data is highly dependent on the environment and skill of the experimenter, and the current ML methods and descriptors are not sufficiently compatible with the diversity of organic synthesis. Therefore, this Research Area aims to build our own digitization platform (**PF**) for digital organic synthesis (interdisciplinary fusion of experimental and information science) that leads to disruptive innovation in organic synthesis.

【Content of the Research Project】

Three Research Groups **A01** (deepening reaction control with AI support), **A02** (deepening synthetic methods with AI support), and **A03** (deepening AI methods to support organic synthesis) will work together to conduct this research (upper right figure). We will develop three automated systems for (1) reaction conditions optimization, (2) synthetic pathway search, and (3) molecular design of highly complex molecules to demonstrate their effectiveness in discovering innovative basic reactions. We will also demonstrate the industrial utility of this PF by (4) developing batch-to-flow conversion methods, (5) constructing automated synthesis systems incorporating an autonomous condition optimization unit, and (6) applying it in multi-step molecular conversion reactions. In addition, we will construct our own database (**DB**) optimized for ML in organic chemistry, which will serve as the basis for the development of automated methods.

The key to promoting research in this area is how to integrate experimental science (synthetic organic chemistry) and information science in a functional manner. It is also important to rapidly accumulate reliable reaction data for ML, and to demonstrate the effectiveness of ML-based predictions through actual experiments. Research Groups A01 and A02 are actively involved in providing data to the DB and using AI and ML. Research Group A03 is working with the experimental group.



【Expected Research Achievements and Scientific Significance】

Driven by information science, we will challenge to create new academic theories through experimental science. First, we will try to super-accelerate the development of innovative reactions such as advanced selectivity control methods. With the help of AI, we will polish the shiny gemstones discovered and put them out into the world. We also introduce objective analysis using AI to reveal a completely new reaction control factor (new principle). We will create the ideal automatic synthesizer by combining a flow-type synthesizer with an in-line analyzer and incorporating an autonomous automatic optimization system for reaction conditions. In the area of information science, we will develop a method (descriptor) for representing molecules and reactions that corresponds to the diversity of organic synthesis, and build a foundation for the digitization of organic synthesis.

【Key Words】

Artificial Intelligence: A program that analyzes characteristics from data and mechanically makes predictions and decisions based on human experience.
Machine Learning: An algorithm that automatically learns to make predictions and decisions through pattern recognition.
Deep Learning: Efficient learning from vast amounts of data using neural networks modeled after human brain circuits.

【Term of Project】

FY2021-2025

【Budget Allocation】

1,155,800 Thousand Yen

【Homepage Address and Other Contact Information】

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