

Realization of common platform technology, facilities, and equipment that creates innovative knowledge and products

Innovation in organic molecular engineering with AI-assisted organic synthesis system using a frugal device

Project Leader : Seijiro MATSUBARA, Professor
Graduate School of Engineering, Kyoto University

R&D Team : National Institute for Material Science, National Institute of Advanced Science and Technology, Tokyo University of Agriculture and Technology



Summary :

The molecular structures, which are devised from material informatics approach (MI), should be converted into the real molecules by organic synthesis in order to obtain new characteristic value. We will develop the AI-assisted automatic system, which can solve the synthetic route of the designed molecule with a suggestion for the reaction conditions. The system synchronizes our newly developing automatic organic synthesis device. Those system means digitization of organic synthesis and will yield a new organic synthesis digital data base. It will also be important for transforming the batch-reactions into the corresponding flow reactions.

