

### Title of Project: Hybrid Catalysis for Enabling Molecular Synthesis on Demand

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### [Purpose of the Research Project]

Organic synthesis has been consistently developed and refined up to the present, but several important issues remain unresolved. One such issue is the practical synthesis of high-value-added complex molecules through streamlined multicatalytic reactions starting from readily-available, abundant molecules. Nature utilizes multicatalytic (i.e., multienzymatic) systems for the biosynthesis of natural products. The most effective artificial multicatalyst system in a flask so far, however, promotes only two or three reactions at most.

With this in mind, the purpose of our research project is to develop hybrid catalysis, a multicatalytic system involving catalysts with distinct individual functions. Integrating the functions of multiple catalysts, hybrid catalysis will enable molecular synthesis of high efficiency, flexibility, and adaptability on demand, starting from abundant organic molecules such as hydrocarbons and other carbon feedstocks (Figure).

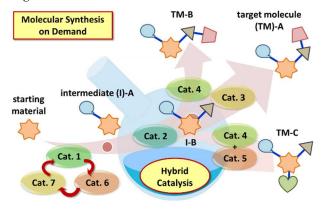


Figure. Molecular Synthesis on Demand Based on the Development of Hybrid Catalysis, Integrating Functions of Multiple Catalysts

### [Content of the Research Project]

Based on the interdisciplinary research ranging from physics to chemistry, we intend to develop conceptually new catalyses leading to innovative organic synthesis. The following three research aspects, A01, A02, and A03, work together to cultivate the supremely high-level research only possible with this project framework.

A01 (Activation): Identification of hybrid catalyses activating stable and abundant organic molecules, including hydrocarbons and other

carbon feedstocks.

A02 (Control): Identification of selective hybrid catalyses that precisely control multiple reaction parameters, including regio-, functional-group, and stereoselectivity, with high flexibility and adaptability.

A03 (Continuity): Identification of domino catalyses rapidly increasing structural complexity, starting from simple molecules to produce multifunctional molecules.

## [Expected Research Achievements and Scientific Significance]

The following ground-breaking achievements are expected: 1) efficient conversion of stable and abundant carbon feedstocks. hydrocarbons, to valuable organic molecules; 2) on-demand synthesis of a specific target molecule among structurally diverse molecules; 3) practical synthesis of target molecules without restriction due to structural complexity. Inducing innovation in molecular synthesis, this project will vastly structural variety of organic expand the molecules available to human beings. This project will markedly influence the various fields that require organic molecules,  $\operatorname{such}$ pharmaceutical sciences, agriculture, and industry. This project will in the long term benefit human healthcare, well-being, and the advancement of civilization and society.

#### Key Words

Hybrid catalysis, molecular synthesis on demand, activation of organic molecules, carbon feedstock, reaction control, regioselectivity, functional-group selectivity, stereoselectivity, domino catalysis, organic synthesis, metal complex catalyst, organocatalyst, solid catalyst, photocatalyst, polymerization catalyst

Term of Project FY2017-2021

**(Budget Allocation)** 1,224,600 Thousand Yen

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