

Report for Interdisciplinary research startup

1. Name of project leader : **Kimichi Suzuki**

2. Project title: 巨大分子系への適用を目指した反応経路自動探索法の開発

Development of automatic reaction path search method for macromolecular systems

3. Report

To make a fusion research theme among organic, medical, theoretical and information researchers come true, we tried to extend the multistructural microiteration method. In previous MSM (-ME) method, an electrostatic interaction between reaction center and surrounding atoms has been treated classically. To describe the interaction quantum mechanically, we have extended to MSM(-EE) method. As a result, MSM-EE gave results in reasonably good agreement with experimental ones, while MSM-ME underestimated barrier height more than 5 kcal mol⁻¹. Based on these results, we considered that our method become one of tools for a reaction design used enzyme and proposed a new theme.

Regarding a budget, we bought a software and using for arrangement of research environment. Especially our development and test calculations promoted due to an installed new software.

4. Research achievement

Conference

1. Kimichi Suzuki and Satoshi Maeda, Development of multistructural microiteration with electronic embedding scheme and its application to Claisen rearrangement reaction (poster)22th Theoretical Chemistry, Hokkaido.
2. Kimichi Suzuki and Satoshi Maeda, Multistructural Microiteration Technique Adopting the Electrostatic Embedding Scheme, (Oral communication), APATCC19, Sydney.
3. Kimichi Suzuki and Satoshi Maeda, Multistructural Microiteration Technique based on the Electrostatic Embedding Scheme, (Invited), 5th Japan-Thai workshop on TCC2019, Yokohama.