

## Report for newly appointed faculty startup

1. Name of project leader : **Yuuya Nagata**

2. Project title: **Development of New Functional Materials Based on the Combination of Theoretical Chemistry and Automated Synthesis**

3. Report

In this study, the applicant has tried to develop new functional materials using theoretical chemistry along with automated synthesis. Firstly, screening of the synthesis of various functional materials was conducted by using the artificial force induced reaction (AFIR) method. Subsequently, preliminary experiments for the synthesis of polymeric materials were conducted according to the results of the theoretical calculations. In order to determine the molecular weight of the obtained compounds, a size exclusion chromatography system was newly introduced owing to the support of ICRéDD (newly appointed faculty startup). Furthermore, the applicant has collaborated with Prof. Varnek group (Prof. Sidorov and Dr. Gimadiev) to develop a database system for chemicals storage in ICRéDD, which is now available and allows us to quickly find chemicals from the storage.

4. Research achievement

Not applicable.