Report for newly appointed faculty startup

1. Name of project leader：**Mikhail Tsitsvero (Prof. Komatsuzaki group)**

2. Project title: **Learning over chemical networks**

3. Report

During the FY2019 I participated in group presentations and meetings on topological data analysis applied to molecular signature matching, modeling of populations over chemical reaction networks and design of suitable differentiable descriptors for learning over chemical reaction networks. Currently I am working on how to quantify the probabilistic uncertainty while performing learning over a set of chemical compounds or chemical reaction network.

4. Research achievement

Group meetings on molecular topology analysis from the perspective of networks, modeling of populations over chemical reaction networks. Currently I am focusing on the design of appropriate differentiable descriptors for learning and fitting of chemical properties using probabilistic framework of Gaussian Processes.