Usage Report for Fiscal Year 2016

**Project Title:**

# Molecular dynamics simulation of virus in water in atomistic resolution

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1. The project goal is to study molecular properties of a virus in water at all atom resolution including explicit water molecules. The study is based on molecular dynamics models of the virus shell (the capsid). We need the Supercomputer for our calculation because full system with the capsid and the water molecules contains few millions atoms and other machines do not allow to perform so heavy simulations.
2. Molecular dynamics simulation using GROMACS.
3. We performed MD simulation of two models of the whole virus, each with two numbers of ions inside of the capsid. Each simulation has been performed for 10 ns in two different force fields: Amber and Gromos.
4. We have concluded that specific distribution of ions inside of the capsid play important role in stability of the capsid.
5. Molecular dynamics simulation of the whole virus with DNA inside. Simulation of the viral self-assembly process.

**Fiscal Year 2016 List of Publications Resulting from the Use of the supercomputer**

**[Publication]**

Tarasova, E.; Farafonov, V.; Khayat, R.; Okimoto, N.; Komatsu, T.; Taiji, M.; Nerukh, D.,
All -Atom Molecular Dynamics Simulations Of Entire Virus Capsid Reveal The Role Of Ion, J. Phys. Chem. Lett., 8 (4), pp 779–784, 2017.
RIKEN is in the authors list of the publication