

34th RAP Seminar

The 34th Seminar on RIKEN Center for Advanced Photonics

Language: Japanese

Date: **June 17 (Fri) 15:30 - 16:30, 2016**

Location: **Cooperation Center, 3F, W319, Wako Campus, RIKEN**

(理研 和光キャンパス 研究交流棟3階会議室 W319)

Title: **Supercomputer Drug Design Based on Physics**

物理法則に基づいたスーパーコンピューター創薬

Speaker: **Prof. Hideaki FUJITANI**

(Research Center for Advanced Science and Technology,
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We perform massively parallel molecular dynamics simulations on large supercomputers in order to design new drugs for pharmaceutical target proteins. Our methods are based on the nonequilibrium statistical physics and quantum physics for biomolecules. We refined AMBER force field by intensive use of high-level quantum mechanics (QM) theory. The dihedral parameters of protein backbone were refined to agree with the torsion energy profiles calculated by high-level QM theory DF-LCCSD(T0) for the model systems of protein backbone. In comparison with conformational preferences of dipeptides in water measured by vibrational spectroscopy, our refined force field (FUJI) produced the best prediction score among the current force fields like AMBER99SB, CHARMM36 and OPLS-AA.