

「分子認識と分子計算」分野 口頭発表
Selected Oral Presentations
(Molecular recognition and molecular modeling)

座長: 石川 岳志 Takeshi Ishikawa (分野長)
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熊澤 啓子 Keiko Kumazawa
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1. [P1-01] Development status of ABINIT-MP program in 2018
 Yuji Mochizuki
 Rikkyo University & The University of Tokyo
2. [P1-07] Effect of Zn on A β Nonamer Aggregates: Molecular Dynamics and
Ab Initio Molecular Orbital Calculation
 Shogo Tomioka
 Toyohashi University of Technology
3. [P1-13] Protein–ligand binding process studied by Markov state model
 Toru Ekimoto
 Yokohama City University
4. [P1-16] Development of the CHARMM force field for Cyclosporine A
 Tsutomu Yamane
 Yokohama City University
5. [P1-19] Structural basis for pH-dependent ferric ion coordination modes of
 TtFbpA, the periplasmic subunit of an ABC-type iron transporter from *Thermus*
thermophilus HB8
 Peng Lu
 The University of Tokyo
6. [P1-20] How proteins recognize a phosphorylated amino acid: Comparative studies
 of an antibody and the other protein families
 Raji Kawade
 The University of Tokyo
7. [P1-21] Non-empirical Coarse-grained Simulations for Lipid Bilayers and Proteins
 Koji Okuwaki
 Rikkyo University
8. [P1-24] FMO Study on the Effects of Phosphorylation in Janus Kinase (JAK) on
 Ligand Binding
 Takahiro Hirata
 Kobe University