FS-22

日時: 2019 年 10 月 23 日　14:30-16:00
場所: 平安

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

モデレーター: **石川 岳志**　Takeshi Ishikawa （分野長）
鹿児島大学 大学院理工学研究科
Kagoshima University, Graduate School of Science and Engineering

山岸 賢司 Kenji Yamagishi
日本大学工学部 生命応用化学科
Nihon University, College of Engineering, Department of Chemical Biology and Applied Chemistry

熊澤 啓子 Keiko Kumazawa
帝人ファーマ株式会社
TEIJIN PHARMA LIMITED

渡邊 博文 Hirofumi Watanabe
神戸大学　計算科学教育センター
Kobe University, Education Center on Computational Science and Engineering

岡田 晃季 Akitoshi Okada
日本たばこ産業株式会社　医薬総合研究所
Central Pharmaceutical Research Institute, JAPAN TOBACCO INC.

口頭発表演題（1演題 10 分:発表　7 分、質疑応答　3 分）

1. [P1-22] A binding free energy calculation method along a modified thermodynamic path which avoids exhaustive enumeration of multiple protein-ligand poses
   Yoshitake Sakae
   Research Organization for Information Science and Technology

2. [P1-28] Advanced methods to predict the property of cyclic peptides: exhaustive and efficient conformation search
   Kentaro Takai
   Fujitsu Ltd.

3. [P1-29] Conformational Changes and Interactions of Calcium Ion Signal Transfer Protein Calmodulin and Calmodulin-binding Domain by Multi-scale and Docking Simulation
   Hiromitsu Shimoyama
   Kitasato University

4. [P1-30] Autoencoder-based Analyses of Dynamic Allostery on Proteins by

Regulator Binding
Yuko Tsuchiya
AIRC, AIST

5. **[P1-33] Computational approaches to drug-receptor binding kinetics**
   Osamu Ichihara
   Schrödinger K.K.

6. **[P1-39] Thermodynamic, kinetic and computational analyses of the recognition mechanism of a flexible protein antigen by an antibody**
   Ikuho Kaneda
   The University of Tokyo

7. **[P1-40] Ligand Binding Mechanism of an Enzyme Studied by Binding Free Energy Analyses for Mutants of the Protein**
   Yoshiharu Mori
   Kitasato University

8. **[P1-47] Interaction Analysis between HEL and HyHEL10 by Fragment Orbital Method**
   Norihito Kawashita
   Kindai University