FS-22

日時: 2019 年 10 月 23 日　16:30-18:00
場所: 平安

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

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口頭発表演題（1演題 10 分:発表　7 分、質疑応答　3 分）

1. [P1-01] Development status of ABINIT-MP program in 2019
   Yuji Mochizuki
   Rikkyo University

2. [P1-03] Binding Energy Calculation of Protein-Peptide Complex Using Unbiased MD Simulations and MSM Analysis
   Hiroaki Hata
   Tokyo Institute of Technology

3. [P1-04] Interaction Analyses between Calcite/Apatite and Peptides by Fragment Molecular Orbital Method
   Ryo Hatada
   Rikkyo University

4. [P1-05] Fragment Molecular Orbital Method Applied to Factor Xa Inhibitors
   Kazufumi Ohkawa
   Asahi Kasei Pharma Corporation

5. **[P1-08] Regulation mechanism of agonistic / antagonistic activities of vitamin D receptor analyzed by generalized ensemble method**
   Takafumi Kudo
   Yokohama City University

6. **[P1-12] Development of the CHARMM force field for Cyclosporine A and application to molecular dynamics simulations using a membrane-water system**
   Tsutomu Yamane
   Yokohama City University

7. **[P1-20] Selectivity of phosphodiesterase-10A inhibitor for phosphodiesterase family elucidated by free energy perturbation approach**
   Toru Ekimoto
   Yokohama City University

8. **[P1-21] *De Novo* Binding Prediction using gREST**
   Suyong Re
   RIKEN BDR