



P01-06 (F-2)

Comparison of molecular dynamics of cyclosporin A and cyclosporin E

Akari Ito

Graduate School of Medical Life Science, Yokohama City
University

Toru Ekimoto

Graduate School of Medical Life Science, Yokohama City
University

Tsutomu Yamane

Center for Computational Science, RIKEN

Mitsunori Ikeguchi

Graduate School of Medical Life Science, Yokohama City
University, and Center for Computational Science, RIKEN



Excellent Poster Awards

P01-09 (F-2)

Activation Pathway of IL-2-inducible T cell kinase Explored by Tree-Search Molecular Dynamics

Yukina Nakai

Yokohama City University

Toru Ekimoto

Graduate School of Medical Life Science, Yokohama City University

Tsutomu Yamane

Center for Computational Science, RIKEN

Naoki Ogawa

Graduate School of Medical Life Science, Yokohama City University

Kei Terayama

Graduate School of Medical Life Science, Yokohama City University

Mitsunori Ikeguchi

Graduate School of Medical Life Science, Yokohama City University



Excellent Poster Awards

P01-12 (F-3)

MDContactCom: A tool to identify differences of protein molecular dynamics from two MD simulation trajectories in terms of residue-residue contacts

Chie Motono

Cellular and Molecular Biotechnology Research Institute, National Institute of Advanced Industrial Science and Technology (AIST)

Shunsuke Yanagida

Bioscience & Healthcare Engineering Div., Mitsui Knowledge Industry Co.

Miwa Sato

Bioscience & Healthcare Engineering Div., Mitsui Knowledge Industry Co.

Takatsugu Hirokawa

Division of Biomedical Science, Faculty of Medicine, University of Tsukuba



Excellent Poster Awards

P02-05 (F-3)

Dynamic FMO analysis for RNA sequence specificity in inhibitor recognition of translation initiation factor complex

Yuma Handa

School of Pharmacy and Pharmaceutical Sciences, Hoshi University

Yusuke Kawashima

School of Pharmacy and Pharmaceutical Sciences, Hoshi University

Takayuki Furuishi

School of Pharmacy and Pharmaceutical Sciences, Hoshi University

Etsuo Yonemochi

School of Pharmacy and Pharmaceutical Sciences, Hoshi University

Takuhiro Ito

Laboratory for Translation Structural Biology, RIKEN Center for Biosystems Dynamics Research

Hironori Saito

RIKEN Cluster for Pioneering Research (CPR) , Department of Computational Biology and Medical Sciences, Graduate School of Frontier Sciences, The University of Tokyo

Shintaro Iwasaki

RIKEN Cluster for Pioneering Research (CPR) , Department of Computational Biology and Medical Sciences, Graduate School of Frontier Sciences, The University of Tokyo

Chiduru Watanabe

Laboratory for Structure-Based Molecular Design, RIKEN Center for Biosystems Dynamics Research

Teruki Honma

Laboratory for Structure-Based Molecular Design, RIKEN Center for Biosystems Dynamics Research

Kaori Fukuzawa

School of Pharmacy and Pharmaceutical Sciences, Hoshi University, Tohoku University Graduate School



Excellent Poster Awards

P03-04 (F-4)

**Design and Implementation of New
Methods for Odor Molecule Generation**

Sijie Zhang

School of Computing, Tokyo Institute of Technology

Masaya Otake

Corporate Research & Development Division, Takasago International Corporation

Hideki Miyazaki

Corporate Research & Development Division, Takasago International Corporation

Kunihide Hoshino

Corporate Research & Development Division, Takasago International Corporation

Takashi Ishida

School of Computing, Tokyo Institute of Technology



Excellent Poster Awards

P03-08 (F-4)

**Development of a Prediction Method
for Protein Cryptic Sites Using Machine
Learning**

Masahito Kumada

the University of Tokyo (Graduate in September 2021)



Excellent Poster Awards

P09-06 (F-7)

Interaction Analysis of GPCR in the Presence of Lipid Bilayer Using Fragment Molecular Orbital (FMO) Method

Taro Imahiro

Hoshi University

Yuma Handa

Hoshi University

Yusuke Kawashima

Hoshi University

Koji Okuwaki

Hoshi University, Rikkyo University

Takayuki Furuishi

Hoshi University

Etsuo Yonemochi

Hoshi University

Kaori Fukuzawa

Hoshi University



Excellent Poster Awards

P09-08 (F-7)

Inhibitor discovery targeting UHRF1 by MD simulations and biochemical analyses

Yuki Shibahashi

Graduate School of Medical Life Science, Yokohama City University

Toru Ekimoto

Graduate School of Medical Life Science, Yokohama City University

Satomi Kori

Graduate School of Medical Life Science, Yokohama City University

Tsutomu Yamane

Center for Computational Science, RIKEN

Kyohei Arita

Graduate School of Medical Life Science, Yokohama City University

Mitsunori Ikeguchi

Graduate School of Medical Life Science, Yokohama City University,
and Center for Computational Science, RIKEN



Excellent Poster Awards

P13-01 (F-7)

In silico-guided design of growth factor mutants with varied physicochemical parameters

Okada Yuga

The University of Tokyo

Eguchi Akihiro

The University of Tokyo

Kuroda Daisuke

The University of Tokyo

Ueki Ryosuke

The University of Tokyo

Sando Shinsuke

The University of Tokyo