



P02-04

**Amino acid preference mapping
on protein-protein interaction
surface using mixed-solvent
molecular dynamics**

Genki KUDO¹, Keisuke

YANAGISAWA², Ryunosuke

YOSHINO^{3, 4}, Takatsugu HIROKAWA^{3, 4}

¹Physics Department, Graduate School of Pure and Applied Sciences, University of Tsukuba, ²Department of Computer Science, School of Computing, Tokyo Institute of Technology, ³Faculty of Medicine, University of Tsukuba, ⁴Transborder Medical Research Center, University of Tsukuba



Excellent Poster Awards

P01-01

Cyclosporin A: Conquering Conformational Complexity and Chameleonicity

Satoshi ONO¹, Matthew R. NAYLOR², Chad
E. TOWNSEND², Chieko OKUMURA¹,
Okimasa OKADA¹, Hsiau-Wei LEE², R.
Scott LOKEY²

¹Discovery Technology Laboratories, Innovative
Research Division, Mitsubishi Tanabe Pharma
Corporation, ²Department of Chemistry and
Biochemistry, University of California Santa Cruz



Excellent Poster Awards

P01-05

**QM/MM simulations of artificial
ion channel in membrane-water
system**

Mayuko NAKAGAWA¹, Toru EKIMOTO¹,
Tsutomu YAMANE², Kohei SATO³, Kazushi
KINBARA³, Mitsunori IKEGUUCHI^{1, 2}

¹Graduate School of Medical Life Science, Yokohama
City University, ²Center for Computational Science,
RIKEN, ³School of Life Science and Technology, Tokyo
Institute of Technology



Excellent Poster Awards

P03-12

**Protein-ligand complex
structure generation with
diffusion-based generative
models**

**Shuya NAKATA, Yoshiharu MORI,
Shigenori TANAKA**

**Graduate School of System Informatics, Kobe
University**



Excellent Poster Awards

P04-01

Computational search for
compounds exhibiting the same
activity from database by
molecular fingerprints and 3D
pseudo-atom methods

Mizuki MATSUSHITA¹, Yuka

YAMASHITA¹, Koji UMEZAWA^{1, 2}

¹Grad. Sch. of Sci. & Tech., Shinshu
University, ²Institute for Biomedical Sciences,
Shinshu University



Excellent Poster Awards

P06-03

**Application of Deep Learning to
the Evaluation of Seizure-like
Behavior Using Zebrafish**

**Mizuho WAKASA¹, Riki KAJIWARA²,
Kaori ABE¹**

¹Department of Investigative Toxicology, Nonclinical Research Center, Tokushima Research Institute, Otsuka Pharmaceutical Co., Ltd., ²Department of Research Management, Otsuka Pharmaceutical Co., Ltd.



P08-07

**AI-AAM. Downsizing and
scaffold hopping from a peptide
to small-molecule inhibitors**

**Shino OHIRA, Jun NAKABAYASHI,
Kyosuke TSUMURA, Issei DOI**

Analysis Technology Center, FUJIFILM corporation



Excellent Poster Awards

P08-11

Estimation of Interaction Mechanism in Compound- Protein Interaction Prediction Using Interpretable Deep Learning

Sota INOUE¹, Shoichi ISHIDA², Iwata
HIROAKI¹, Matsumoto SHIGEYUKI¹,
Kojima RYOSUKE¹, Okuno YASUSHI¹

¹Graduate School of Medicine, Kyoto
University, ²Graduate School of Medical Life Science,
Yokohama City University



Excellent Poster Awards

P08-15

Understanding Molecular Mechanism of Drug Off-Target Effect in Tyrosine-Protein Kinase LCK Using Molecular Dynamics Simulation

Hidetoshi TAGE¹, Shigeyuki
MATSUMOTO¹, Hiroaki IWATA¹, Yuta
ISAKA², Biao MA², Mitsugu ARAKI¹,
Atsushi TOKUJHISA², Ryo KANADA²,
Yasushi OKUNO^{1, 2}

¹Graduate School of Medicine and Faculty of
Medicine, Kyoto University, ²Riken Center for
Computational Science



P08-19

**Automated hetero shuffling
combined with FMO
calculations**

**Sundaram ARULMOZHIRAJA,
Kazufumi OHKAWA**

Asahi Kasei Pharma