

# Excellent Presentation Award

**001-02**

**GLDADec: Guided LDA deconvolution enabled us to identify cell type proportion**

**Iori AZUMA, Tadahaya MIZUNO, Hiroyuki KUSUHARA**

Laboratory of Molecular Pharmacokinetics, Graduate School of Pharmaceutical Sciences,  
The University of Tokyo

**002-04**

**Application of Machine Learning Models in Prediction of Disease Therapeutic Target Molecules Using Gene Expression Profiles**

**Narumi HATANO<sup>1</sup>, Mayumi KAMADA<sup>1</sup>, Ryosuke KOJIMA<sup>1</sup>, Hiroaki IWATA<sup>1</sup>, Yasushi OKUNO<sup>1, 2</sup>**

<sup>1</sup>Graduate School of Medicine and Faculty of Medicine Kyoto University,  
<sup>2</sup>RIKEN Center for Computational Science (R-CCS)HPC/HPC- and AI-driven Drug Development Platform Divisio

**O03-01**

**De novo inhibitor and activator design from gene expression profiles via deep learning and Bayesian optimization**

**Yuki MATSUKIYO<sup>1</sup>, Chikashige YAMANAKA<sup>1</sup>, Yoshihiro YAMANISHI<sup>1, 2</sup>**

<sup>1</sup> Department of Bioscience and Bioinformatics, Faculty of Computer Science and Systems Engineering, Kyushu Institute of Technology, <sup>2</sup> Graduate School of Informatics, Nagoya University

**O04-04**

**Study Improves Performance of Pocket Comparisons Using Machine Learning**

**Risa SHIOZAWA, Masakazu SEKIJIMA, Nobuaki YASUO**

Tokyo Institute of Technology

**O05-02**

**Structural and Computational Insight into  
Dynamics and Intermediate State in Activation of  
Orexin 2 Receptor**

**Shun YOKOI<sup>1, 2</sup>, Ayori MITSUTAKE<sup>1</sup>**

<sup>1</sup>Department of Physics, School of Science and Thechnology, Meiji University, <sup>2</sup>Structural Biology Department, School of Medicine, Stanford University

**O06-06**

**Transformer Encoder-based Generative  
Adversarial Network for Design of  
Polypharmacological Drugs**

**Kasumi YASUDA<sup>1</sup>, Chen LI<sup>1, 2</sup>, Kazuma KAITOH<sup>1, 2</sup>, Yoshihiro YAMANISHI<sup>1, 2</sup>**

<sup>1</sup>Department of Bioscience and Bioinformatics, Faculty of Computer Science and Systems Engineering, Kyushu Institute of Technology, <sup>2</sup>Graduate School of Informatics, Nagoya University

**O07-06**

## **AdaSplit: an adaptive dataset split method**

**Nathan Robert LUGG, Thomas PEACOCK, Joel C FORSTER,  
Ross Henry JOHNSTONE, Benjamin INGLEDOW, Koki  
SHIMADA**

SyntheticGestalt

**O08-05**

## **High-Resolution AFM Imaging of DNA Structures: An Approach via Cycle GANs and Virtual Reality Integration**

**Xiaoran HU<sup>1, 3</sup>, Qing LIU<sup>2</sup>, Gregory GUTMANN<sup>3</sup>, Masayuki  
YAMAMURA<sup>1</sup>, Akinori KUZUYA<sup>2</sup>, Akihiko KONAGAYA<sup>3, 4, 5</sup>**

<sup>1</sup>Tokyo Institute of Technology, <sup>2</sup>Kansai University, <sup>3</sup>Molecular  
Robotics Research Institute, Co., Ltd, <sup>4</sup>Keisen University, <sup>5</sup>CBI  
Research Institute