



Best Poster Award

P10-19

Tatsuya Yoshizawa

Graduate School of Medical Life Science,
Yokohama City University

**Molecule Generation with Boltz-2: A Case Study on
Kinase Inhibitor Design**



CBI2025 Like! Poster Award

P10-02

Akitoshi Okada

Daiichi Sankyo Co., Ltd.

**Boltz2 benchmark on in-house dataset: thinking of
how to effectively use in drug discovery campaigns**



Excellent Poster Awards

P01-04

Chie Motono

National Institute of Advanced Industrial Science
and Technology (AIST)

**CrypTothML: A Hybrid MD–ML Approach for
Cryptic Site Prediction**

P01-18

Yuta Kawaura

Kyushu University

**Predicting Protein-Ligand Binding Affinity via
Markov State Modeling and Fragment Molecular
Orbital Analysis**

P02-04

Takamasa Suzuki

Institute of Science Tokyo

Development of a de novo molecular generative model using decoupled setting in multi-objective Bayesian optimization

P03-05

Ryoya Kawabata

Osaka Metropolitan University

Electron Density Topography (EDT) Based on Middle-Angle X-ray Scattering Data Reveals Novel Structural Insights into MAP2K6 and p38 α MAPK in solutions

P04-09

Soyoka Tanihata

Tottori University

Modeling Ethnic Differences in Drug Clearance via Predicted Pharmacokinetics from Chemical Structures

P05-05

Kodai Miyazaki

School of Pharmaceutical Sciences, University of
Shizuoka

**Identification of Cancer-Associated Fibroblast
Subtypes That Promote HCC Progression and
Their Differentiation Programs**

P06-02

Seisuke Takimoto

JAPAN TOBACCO INC.

Initiatives for predict-first DMTA cycle in JT

P06-06

Masami Sako

Institute of Science Tokyo

**DiffPharma : A Conditional Diffusion Framework
for Interaction-Constrained 3D Molecular Design**

P07-03

Hayato Nakahara

Tottori university

Development and Evaluation of a Machine Learning Model for Classifying Neurodegenerative Diseases from Transcriptomic and GO Data

P08-03

Reo Toho

Department of Applied Chemistry, Graduate School of Engineering, Mie University

DNA Origami Nanoactuators for Stimulus-Responsive and Programmable Liposome Shape Control

P10-21

Yuki Satoh

ONO PHARMACEUTICAL CO., LTD

REINVENT4 Ecosystem and LLM-Powered Patent Analysis Tool: OSS Implementation with Case Studies