

**「インシリコ創薬」分野 口頭発表****Selected Oral Presentations****(*In silico* drug discovery)**

**座長:** 池田 和由 Kazuyoshi Ikeda  
慶應義塾大学薬学部 Keio University

1. [P2-14] A Concept of Automated Lead Optimization Method by Compound Property Enhancement and Learning to Rank  
Nobuaki Yasuo  
Tokyo Institute of Technology
2. [P2-01] Design of Anti-Cancer Peptides with Counterpropagation Artificial Neural Networks  
Miyabi Hishinuma  
Tokyo Institute of Technology
3. [P2-18] Subtype specificity analysis of estrogen receptor using fragment molecular orbital method  
Yuya Seki  
Hoshi University
4. [P2-03] Structure Information Management System in Asahi Kasei Pharma  
Kazufumi Ohkawa  
Asahi Kasei Pharma Corporation
5. [P2-05] Bandit Ensemble FMO for Protein-Ligand Binding Affinity Predictions  
Kenichiro Takaba  
Asahi Kasei Pharma Corporation
6. [P2-23] Data Analysis Toolkits of Fragment Molecular Orbital Calculations to Visualize Interaction Energies Using the GUI Plugin for PyMOL  
Takaki Tokiwa  
Tohoku University
7. [P2-16] Statistical analysis of inter- and intramolecular interactions for drug design based on FMO database  
Chiduru Watanabe  
RIKEN Center for Biosystems Dynamics Research
8. [P2-04] Implementation of protein-ligand docking engine sievгене\_M for many- and multi-core processors  
Takanori Sugihara  
Japan Biological Informatics Consortium