Best Poster Award

P07-02

Automation of building ML prediction models using in-house data and development of prediction result response applications

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Excellent Poster Award

P01-10

Applicabilities of Neural Network Potential to Predict ligand-RNA Interactions

 $\underline{Hiroto\ ASANO^1},\ Hiromu\ MATSUMOTO^2$, Shu $OHNO^1$, Yuma $HANDA^{1,\,3},\ Asuka\ HATABU^1$, Daisuke $TAKAYA^1$, Kenji $IKEDA^1$, Yu-Shi $TIAN^1$, Kaori $FUKUZAWA^1$, Kato $KOICHIRO^2$

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P02-11

Comprehensive structual analysis of PROTAC mediated ternary complexes using enhanced conformational sampling methods

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P03-06

Computational-Model-Based Machine-Learning Prediction of Regioselectivity in Organic Reactions: Application to Electrophilic Attach to Quinone Derivatives

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P03-11

Investigation on the Transformer's learning process of chemical structure comprehension

<u>Yasuhiro YOSHIKAI</u>, Tadahaya MIZUNO, Hiroyuki KUSUHARA

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

P04-02

Development of effi cient process to extract SAR knowledge from literature by using CCR algorithm

Kosuke TAKEUCHI, Takayuki SERIZAWA, Takahisa SHIMIZU, Shuhei UESUGI

Medicinal Chemistry Research Laboratories, DAIICHI SANKYO CO., LTD.

P06-06

Identifying suitable AlphaFold2 protein structure models for improved structure-based virtual screening

Keisuke UCHIKAWA, Kairi FURUI, Masahito OHUE

Department of Computer Science, School of Computing, Tokyo Institute of Technology

P08-10

PROTAC molecular linker design using fragment linking method

Ryota ISHIZAWA, Masahito OHUE

Department of Computer Science, School of Computing, Tokyo Institute of Technology

P08-15

Application of Parallel Cascade Selection
Molecular Dynamics for generating virtual
screening models

<u>Takumi HIRAO</u>¹, Genki KUDO², Yoshino RYUNOSUKE^{3,4}, Takatsugu HIROKAWA^{3, 4}

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P09-04

A Graph Based Method of Pattern Mining for Spatial Transcriptome Data

<u>Ayaka MAE</u> ¹, Shigeto SENO¹, Hironori SHIGETA¹, Yu-Chen LIU², Sangeun KIM³, Daisuke OKUZAKI², Ryoichi MORI³, Hideo MATSUDA¹ ¹ Graduate School of Information Science and Technology, Osaka University, ² WPI Immunology Frontier Research Center, Osaka University, ³ Graduate School of Biomedical Sciences, Nagasaki University

P10-04

Establishment of the precise early prediction models of low-birth-weight for term and preterm birth groups based on genetic and environmental factors

Satoshi MIZUNO¹, Satoshi NAGAIE¹, Gen TAMIYA¹, Shinichi KURIYAMA¹, Taku OBARA¹, Mami ISHIKURO¹, Hiroshi TANAKA², Kengo KINOSHITA¹, Junichi SUGAWARA¹, Masayuki YAMAMOTO¹, Nobuo YAEGASHI¹, Soichi OGISHIMA¹

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P10-08

Elucidation of Mortality Triggers Using Temporal Predictive Models $\underline{Tatsuki\ YAMAMOTO^1},\ Yuzuha\ TSUJI^2$, Minoru SAKURAGI^2, Yuji OKAMOTO^2, Mayumi KAMADA^2, Yasushi OKUNO^2

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