

Program

Wednesday, November 16

9:00 – Registration

Opening Remarks

9:50 – 10:00

Yoshiaki NAKAGAWA

Oral Presentation

10:00 – 10:40

Chairperson: Teruki HONMA

KO-01 *Analysis of the ligand-receptor binding for various molting hormone agonists using molecular dynamics* 17

○Shinri Horoiwa, Masahiro Miyashita, Yoshiaki Nakagawa and Hisashi Miyagawa
(Graduate School of Agriculture, Kyoto University)

KO-02 *Stereospecific inhibition of nitric oxide production in macrophage cells by flavanonols: Synthesis and the structure-activity relationship 2* 19

○Wen-Jun JIANG, Tomoko TAKAMIYA, Susumu KITANAKA, Hiroshi IJIMA
(School of Pharmacy, Nihon University)

Invited Lecture

10:50 – 11:30

Chairperson: Kazunari HATTORI

I-01 *Supercomputer and big data driven drug discovery* 4

○Yasushi Okuno
(Graduate school of Medicine, Kyoto University)

11:30 – 12:10

Chairperson: Nobuyuki OKAJIMA

I-02 *Computer-aided drug design software myPresto for rational structure-guided drug development* 6

○Yoshifumi FUKUNISHI
(National Institute of Advanced Industrial Science and Technology & Technology
Research Association for Next-Generation Natural Products Chemistry)

Luncheon Seminar

Affinity Science
Kyoto Constella Technologies

Invited Lecture

13:20 – 14:00

Chairperson: Fumiyoshi YAMASHITA

I-03 *Development of a new QSAR analysis method to study drug-drug interactions of human ABC transporters: Application to drug discovery and cancer therapy*8

○Toshihisa ISHIKAWA^{1,2}, Hikaru SAITO¹, Hiroyuki HIRANO¹

(¹Tokyo Institute of Technology, ²NGO Personalized Medicine & Healthcare)

Special Session

14:00 – 14:40

Chairperson: Miki AKAMATSU & Hiroshi TERADA

SL-01 *Computer-aided molecular design: From QSAR to pharmacophore-based ligand profiling*3

○Thierry LANGER

(Department of Pharmaceutical Chemistry, University of Vienna, Althanstrasse 14, 1090 Vienna, Austria)

Poster Presentation

14:50 – 15:50 (Poster presentations with odd numbers)

15:50 – 16:50 (Poster presentations with even numbers)

Symposium on Structure-Activity Relationship

KP-01 *A quest for novel chymase inhibitors by 3D pharmacophore-based virtual screening* 33

○Shin-ichiro OZAWA, Shoichi ISHIDA, Maho HABUKA, Shuichi HIRONO
(School of Pharmacy, Kitasato University)

KP-02 *Energy-based analysis and prediction of peptide-HLA interactions* 35

○Daisuke KURODA, Hiroaki GOUDA
(Department of Analytical and Physical Chemistry, Showa University School of Pharmacy)

KP-03 *Estimations of selectivities of opioid agonists using three 3D-QSAR models based on each alignment of molecules docked into μ , κ , and δ -opioid receptors* 37

○Noriyuki YAMAOTSU, Shuichi HIRONO
(School of Pharmacy, Kitasato University)

KP-04	<i>A computational study of water-assisted cyclization mechanism of glutamate residue</i>	39
	○Tomoki NAKAYOSHI ¹ , Shuichi FUKUYOSHI ¹ , Ohgi TAKAHASHI ² , Akifumi ODA ^{3,4} (¹ Division of Pharmaceutical Sciences, Graduate School of Medical, Pharmaceutical and Health Sciences, Kanazawa University, Faculty of Pharmaceutical Sciences, ² Tohoku Medical and Pharmaceutical University, ³ Faculty of Pharmacy, Meijo University, ⁴ Institute for Protein research, Osaka University)	
KP-05	<i>Three dimensional structures of primitive proteins generated in the racemic amino acid pool</i>	43
	○Akifumi ODA ^{1,2,3} , Shuichi FUKUYOSHI ³ , Eiji KURIMOTO ¹ (¹ Faculty of Pharmacy, Meijo University, ² Institute for Protein Research, Osaka University, ³ Faculty of Pharmacy, Institute of Medical, Pharmaceutical and Health Sciences, Kanazawa University)	
KP-06	<i>Evaluation of docking program for cytochrome P450: a case of Mycobacterium CYP121</i>	45
	○Miki H. MAEDA (Advanced Analysis Center, National Agriculture and Food Research Organization)	
KP-07	<i>Interaction analyses of CDK2 with its inhibitors by FMO calculation and PLS regression</i>	47
	○Tomoki YOSHIDA, Shuichi HIRONO (School of Pharmacy, Kitasato University)	
KP-08	<i>Analyses of protein – ligand interaction of BACE1 and its ligands using fragment molecular orbital method</i>	49
	○Yuji HASHIMOTO ¹ , Norihito KAWASHITA ^{1,2} , Hiroto MORIWAKI ¹ , Yu-Shi TIAN ³ , Tatsuya TAKAGI ^{1,2} (¹ Graduate School of Pharmaceutical Science, ² Research Institute for Microbial Diseases, ³ Graduate School of Information Science and Technology, Osaka University)	
KP-09	<i>In silico analyses of interactions between hexosaminidase A and its high potent ligands</i>	51
	○Izumi NAKAGOME ¹ , Atsushi KATO ² , Noriyuki YAMAOTSU ¹ , Isao ADACHI ² , Shuichi HIRONO ¹ (¹ Kitasato University, School of Pharmacy, ² Department of Hospital Pharmacy, University of Toyama)	

- KP-10** *Development of the protein 3D fragment analysis system focused on ligand binding loop regions*53
 ○Akihiro HIRAMA, Hiroaki KATO
 (Toyohashi University of Technology)
- KP-11** *Prediction of detailed enzyme functions and identification of specificity determining residues by random forest using information about active sites and enzyme-ligand complex structures*55
 ○Chioko NAGAO¹, Nozomi NAGANO², Kenji MIZUGUCHI¹
 (¹National Institutes of Biomedical Innovation, Health and Nutrition, ²National Institute of Advanced Industrial Science and Technology)
- KP-12** *Prediction of 3D protein-ligand interactions in enzymatic reactions* 57
 ○Yoichi MURAKAMI^{1,4}, Satoshi OMORI¹, Kengo KINOSHITA^{1,2,3}
 (¹Graduate School of Information Sciences, Tohoku University, ²Institute of Development, Aging and Cancer, Tohoku University, ³Tohoku Medical Megabank Organization, ⁴Center for Drug Design Research, National Institutes of Biomedical Innovation, Health and Nutrition)
- KP-13** *Development of the quick federated substructure search (QFSS) method for huge compound database based on the indexing of novel substructure fingerprints* ...59
 ○Seiichi KOBAYASHI, Kinya TODA, Ryoichi KATAOKA, Junichi GOTO
 (Ryoka Systems Inc.)
- KP-14** *Development of the common fragment set extraction system for compound-protein relationship studies*61
 ○Yoshiyuki SATO, Hiroaki KATO
 (Toyohashi University of Technology)
- KP-15** *Prediction of protein complex structures and interfacial water positions by template-based modeling in CAPRI round 34*63
 ○Yasuomi KIYOTA, Yudai YAMAMOTO, Mayuko TAKEDA-SHITAKA
 (School of pharmacy, Kitasato University)
- KP-16** *Synthesis of fluorinated isoxazolines and 5-alkoxyisoxazolines for a biological activity evaluation*65
 ○Kazuyuki SATO,¹ Graham SANDFORD,² Niko YANADA,¹ Atsushi TARUI,¹ Akira ANDO,¹ Masaaki OMOTE¹
 (¹Faculty of Pharmaceutical Sciences, Setsunan University, ²Department of Chemistry, Durham University)

- KP-17** *Analysis for assembling mechanism of coiledcoil domains in yeast cargo receptor Emp46p/47p and modification of pH-dependence for the complex formation* ...67
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 (¹Faculty of pharmacy, Meijo University, ²Institute for protein research, Osaka University)
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 ○Toshiaki TAURA, Naoto FUKUOKA, ○Tomoya NOBUNAGA
 (Faculty of Information Science and Technology, University of Aichi Prefecture)
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 ○Kenichiro FUJII¹, Shuichi FUKUYOSHI¹, Noriyuki YAMAOTSU², Shuichi HIRONO², Akifumi ODA^{3,4}
 (¹Division of Pharmaceutical Sciences, Graduated School of Medical, Pharmaceutical and Health Sciences, Kanazawa University, ²School of Pharmacy, Kitasato University, ³Faculty of Pharmacy, Meijo University, ⁴Institute for Protein Research, Osaka University⁴)
- KP-20** *Presumption of amyloid- β aggregation mechanism based on the structure-activity relationships for aggregation inhibition and docking studies* 75
 ○Riho TAGUCHI, Tomohito TAKAHASHI, Suguru KOSAKA, Kiyotaka TOKURAKU, Koji UWAI
 (Muroran Institute of Technology)
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 ○Ayako FURUHAMA, Takehiko I. HAYASHI, Norihisa TATARAZAKO
 (Centre for Health and Environmental Risk Research, National Institute for Environmental Studies)
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 (¹Optibrium Ltd, ²Hulinks Inc.)
- KP-23** *Fish toxicity prediction of chemicals using TFS-PLS method in conjunction with Active QSAR modeling* 81
 ○Ryota KIKUCHI, Tetsuo KATSURAGI, Yoshimasa TAKAHASHI
 (Department of Computer Science and Engineering, Toyohashi University of Technology)

- KP-24** *Fish toxicity prediction of chemicals using atomic fragment method: refinement of the fragments and improvement of the prediction model* 83
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 (Toyohashi University of Technology)
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 (Graduate School of Agriculture, Kyoto University)
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 (Okayama Univ., Osaka Univ., Nagahama Bio-tec Univ.)
- KP-27** *Computational study of isomerization reaction route of the aspartic acid*
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 ○Shuichi FUKUYOSHI¹, Tomoki NAKAYOSHI¹, Ohgi TAKAHASHI², Akifumi ODA^{3,4}
 (¹Institute of Medical, Pharmaceutical and Health Sciences, Kanazawa University. ²Tohoku Medical and Pharmaceutical University. ³Faculty of Pharmacy Meijo University. ⁴Institute for Protein Research, Osaka University)
- KP-28** *Eigenvector of molecular matrix and atomic environment of molecule*
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 ○Kouhei MURAKAMI, Tetsuo KATSURAGI, Yoshimasa TAKAHASHI
 (Toyohashi University of technology)

Assembly for Pesticide Design Research

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(Kazuo SOENO², Yusuke KAKEI¹, Miho TATSUKI³, [○]Yukihisa SHIMADA¹
¹Yokohama City University, Kihara Institute for Biological Research, ²WARC/NARO, ³NIFTS)
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[○]Tadaaki MASHIMO^{1,2}, Yoshinori WAKABAYASHI³, Mitsuhiro WADA², Yoshifumi FUKUNISHI^{2,4}, Haruki NAKAMURA⁵
(¹IMS BIO Co. Ltd, ²Technology Research Association for Next-Generation Natural Products Chemistry, ³BY-HEX LLP, ⁴molprof, AIST, ⁵Institute for Protein Research, Osaka University)
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 (¹Graduate School of Agriculture, Kyoto University, ²Graduate School of Science, Osaka Prefecture University)
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 (Graduate School of Agriculture, Kyoto University)
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 ○Yuko MORI,¹ Azusa SASAKI,² Kouji KURAMOCHI,¹ Yasushi NAKAMURA²
 (¹Department of Applied Biological Science, Faculty of Science and Technology, Tokyo University of Science, ²Graduate School of Life and Environmental Sciences, Kyoto Prefectural University)
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 ○Tadahiro AKIYAMA¹, Hiroyuki YAMANO¹, Ryunosuke WADA¹, Takuya YAMAGISHI¹, Masaki MORI², Kazunori OKADA³, Tadao ASAMI¹
 (¹Dept. Appl. Biol. Chem, University of Tokyo, ²Institute of Agrobiological Sciences, NARO, ³Biotech. Research Center, University of Tokyo)
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Plenary Lecture

17:00 – 18:00

Chairperson: Yoshiaki Nakagawa

PL-01 *A structural view of allosteric control of transcription by steroid nuclear*

receptors 1

○Isabelle M.L. BILLAS, Bruno P. KLAHOLZ, Dino MORAS

(IGBMC, Centre National de la Recherche Scientifique (CNRS), UMR 7104, Institut National de la Santé et de la Recherche Médicale (INSERM) U964, Université de Strasbourg, Illkirch, 67404, France)

Banquet

18:10 – 20:10 Kyoto University, Shiran Kaikan

Thursday, November 17

Oral Presentation

9:30 – 10:10

Chairperson: Shinji SUNADA

KO-03 *An automated de novo ligand design framework utilizing open source software*
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○Ryuki KUDO, Tomoko ADACHI, Hiroyuki YAMASAKI, Yoshihiko NISHIBATA
(School of Pharmacy, Kitasato University)

KO-04 *Visualization of chemical space and protein space considering compound-protein interaction*
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○Iwao MAEDA, Hiromasa KANEKO, Kimito FUNATSU
(School of Engineering, The University of Tokyo)

10:10 – 10:50

Chairperson: Mayuko TAKEDA-SHITAKA

KO-05 *Structure similarity search using the hierarchy of its NTGs*
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○Tetsuo KATSURAGI, Yoshimasa TAKAHASHI
(Department of Computer Science and Engineering, Toyohashi University of Technology)

KO-06 *Constructing prediction models of adverse drug reactions using machine learning*
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○Hiroaki MORIUCHI¹, Yu-Shi TIAN², Hiroto MORIWAKI¹, Satoshi AOKI³, Nobuki TAKAYAMA³, Norihito KAWASHITA^{1,4}, Takayuki HIBI², Tatsuya TAKAGI^{1,4}
(¹Graduate School of Pharmaceutical Sciences, Osaka University, ²Graduate School of Information Science and Technology, Osaka University, ³Graduate School of Science, Kobe University, ⁴Research Institute for Microbial Diseases, Osaka University)

Invited Lecture

11:00 – 11:40

Chairperson: Hirosato TAKIKAWA

I-04 *Total synthesis of hatch stimulating agents of cyst nematodes*
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○Keiji TANINO
(Faculty of Science, Hokkaido University)

Luncheon Seminar

OpenEye Japan Co., Ltd

Invited Lecture

13:20 – 14:00

Chairperson: Hiromasa KIYOTA

I-05 *Synthesis of azadirachtin, an insect antifeedant*

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○Naoki MORI, Hidenori WATANABE (Graduate School of Agricultural and Life Sciences, The University of Tokyo)

14:00 – 14:40

Chairperson: Masahiro MIYASHITA

I-06 *Protein–ligand interactions studied by molecular simulations*

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○Tohru TERADA, Yoshitaka MORIWAKI, Tatsuki NEGAMI, Kentaro SHIMIZU (Graduate School of Agricultural and Life Sciences, The University of Tokyo)

Invited Lecture

14:50 – 15:30

Chairperson: Masateru OHTA

I-07 *Protein dynamics investigated by a combination of molecular dynamics*

simulations and small-angle x-ray scattering experiments 15

○Mitsunori IKEGUCHI (Graduate School of Medical Life Science, Yokohama City University)

Awards Ceremony

15:30 – 16:00

Closing Remarks

16:00 – 16:05

Yoshiaki NAKAGAWA

Associate Professor, Graduate School of Agriculture, Kyoto University