# シンポジウム　Symposia

**Friday, 22 March　11:00 ~ 12:05 / 14:45 ~ 17:40**

**Plenary Lecture: Room C, International Conference Hall, Makuhari Messe**

**Invited Poster Presentation: Room PO, International Exhibition Hall 8, Makuhari Messe**

## 第 5 回国際創薬シンポジウム　ISMS
## 5th International Symposium for Medicinal Sciences

11:00 ~ 11:05

**Opening Remark**　Chairman: Akira OTAKA（Tokushima University）

11:05 ~ 12:05

**Plenary Lecture 1**　Chairman: Yoshio HAYASHI（Tokyo University of Pharmacy and Life Sciences）

**ISMS-PL01**　Attacking the Cell Surfaceome in Cancer
James A. WELLS（Department of Pharmaceutical Chemistry, University of California）

14:45 ~ 15:45

**Plenary Lecture 2**　Chairman: Daisuke TANAKA（Exscientia Ltd.）

**ISMS-PL02**　The AI Revolution in Drug Discovery
Andrew L. HOPKINS（Exscientia Ltd.）

16:00 ~ 17:40

**Invited Poster Presentation**

**Odd Number:　16:00 ～ 16:50**
**Even Number: 16:50 ～ 17:40**

**ISMS-IP01**　Clinical Evidence-based Drug Repositioning and Target Discovery
○ Shuji KANEKO[1], Takuya NAGASHIMA[1]（[1]Department of Molecular Pharmacology, Graduate School of Pharmaceutical Sciences, Kyoto University）

**ISMS-IP02**　New Insights for Drug Repositioning: the Integrative Approach
○ Lili MAO[1], Mai FUJIMOTO[2], Kouichi HOSOMI[2], Mitsutaka TAKADA[2], Juran KATO[1]
（[1]GEXVal Inc., [2]Division of Clinical Drug Informatics, School of Pharmacy, Kindai University）

**ISMS-IP03**　Development of Acyl Transfer-based Chemical Biology Tools for Purification/Selective Labeling of Target Proteins
○ Akira SHIGENAGA[1], Takuya MORISAKI[1], Taiki KOHIKI[1], Masaya DENDA[1], Tsubasa INOKUMA[1], Akira OTAKA[1]（[1]Institute of Biomedical Sciences and Graduate School of Pharmaceutical Sciences, Tokushima University）

**ISMS-IP04**　Selective Degradation of Splicing Factor CAPER$\alpha$ by Anticancer Sulfonamides
○ Taisuke UEHARA[1], Yukinori MINOSHIMA[1], Koji SAGANE[1], Naoko HATA SUGI[1], Kaoru OGAWA MITSUHASHI[1], Noboru YAMAMOTO[1], Hiroshi KAMIYAMA[1], Kentaro TAKAHASHI[1], Yoshihiko KOTAKE[1], Mai UESUGI[1], Akira YOKOI[1], Atsushi INOUE[1], Miyuki MABUCHI[2], Akito TANAKA[2], Takashi OWA[1]（[1]Eisai Co., Ltd., [2]School of Pharmacy, Hyogo University of Health Science）

**ISMS-IP05**　Target-selective Degradation of Intracellular Molecules via Autophagy
○ Daiki TAKAHASHI[1], Jun MORIYAMA[1], Erika MIKI[1], Tomoe NAKAMURA[1], Ayami SATO[1], Kaori ITTO-NAKAMA[1], Hirokazu ARIMOTO[1]（[1]Graduate School of Life Sciences, Tohoku University）

**ISMS-IP06** Investigation of the Chemical Space for Brain Penetrable, Carboxylic Acid-containing Compounds: Expanding the Area Available for CNS Drug Discovery

○ Yoshiaki OHASHI[1] ([1]Medicinal Chemistry, Neurology Tsukuba Research Department, Discovery, Medicine Creation, Neurology Business Group, Eisai Co., Lid.)

**ISMS-IP07** Interaction Analysis between MDM2 and Its Inhibitors by Fragment Molecular Orbital Method

○ Norihito KAWASHITA[1], Naoto MOTOYAMA[2], Tian YU-SHI[2], Hirotomo MORIWAKI[2], Tatsuya TAKAGI[2] ([1]Faculty of Science and Engineering, Kindai University, [2]Graduate School of Pharmaceutical Sciences, Osaka University)

**ISMS-IP08** SEEDSUPPLY Contributes to Maximizing the Values of Small Molecule Drug Discovery

○ Takashi MOTOYAJI[1] ([1]SEEDSUPPLY INC.)

**ISMS-IP09** A Prediction Framework for Drug Discovery Using Graph Convolutional Networks

○ Ryosuke KOJIMA[1] ([1]Department of Biomedical Data Intelligence, Graduate School of Medicine, Kyoto University)

**ISMS-IP10** Autodesign – an Automated Drug Design by Using Molecular Simulation Data of Protein-ligand Systems

○ Hironori KOKUBO[1], Naoki MIYAMOTO[1], Yoshi NARA[1], Sachiko ITONO[1] ([1]Axcelead Drug Discovery Partners, Inc.)

**ISMS-IP11** Generation of Chemical Structures with a Desired Pharmacophore Using Deep Reinforcement Learning

○ Atsushi YOSHIMORI[1], Enzo KAWASAKI[2], Chisato KANAI[2], Tomohiko TASAKA[3]([1]Institute for Theoretical Medicine, Inc., [2]Kyoto Constella Technologies Co., Ltd, [3]Affinity Science Corp.)

**ISMS-IP12** Chemical Data Science for Drug Design: New Development of the KY-methods in Big Data Era

○ Kohtaro YUTA[1] ([1]In Silico Data, Ltd.)

**ISMS-IP13** Development of Fluorescent Probes for Exopeptidases for Realizing Novel Medical Imaging

○ Yugo KURIKI[1], Mako KAMIYA[2,3], Toru KOMATSU[1], Yasuteru URANO[1,2,4] ([1]Grad. Sch. Pharm. Sci., [2]Grad. Sch. Med., The Univ. of Tokyo, [3]JST PRESTO, [4]AMED CREST)

**ISMS-IP14** Artificial Chemical Transformation of Amyloid Peptide by Catalytic Photo-Oxygenation

○ Youhei SOHMA[1], Jizhi NI[1], Atsuhiko TANIGUCHI[1,2], Shuta OZAWA[1], Yukiko HORI[1], Taisuke TOMITA[1], Motomu KANAI[1] ([1]Graduate School of Pharmaceutical Sciences, The University of Tokyo, [2]Tokyo University of Pharmaceutical and Life Sciences)

**ISMS-IP15** Potential of Imaging Mass Spectrometry in Neurotransmitter-driven Drug Discovery

○ Kenichi WATANABE[1], Jun TADANO[1], Toichiro YAMADA[1], Tetsuya NAKAGAWA[1], Izuru MIYAWAKI[1] ([1]Sumitomo Dainippon Pharma Co.,Ltd.)

**ISMS-IP16** Screening of Food Materials and Drugs that Can Suppress Cardio Sudden Death by Lipid Peroxidation Using Heart Specific GPx4 KO Mice

○ Tomoko KOUMURA[1], Hirotaka IMAI[1] ([1]School of Pharmaceutical Sciences, Kitasato University)

**ISMS-IP17** Long-Lasting Effect of Allergen-Specific Sublingual Immunotherapy is Dose and Duration Dependent in a Murine Allergic Rhinitis Model

○ Soichi TOFUKUJI[1] ([1]Drug Discovery & Disease Research Laboratory, Shionogi & Co., Ltd.)

**ISMS-IP18** Recent Progress in the Development of Microphysiological Systems and Their Implementation at Astellas

○ Kazuhiro TETSUKA[1], Masato OHBUCHI[1], Tetsuhiro KAWABE[1], Takayuki GOTO[1], Fumiko KIYONAGA[1], Kaori TAKAMA[1], Shunji YAMAZAKI[1], Akira FUJIMORI[1] ([1]Drug Discovery Research, Astellas Pharma Inc.)

**ISMS-IP19** Docetaxel might be Preferable Combination Partner for Immunotherapy

○ Miya HARUNA[1,2], Yoko YAMAMOTO[2], Michinari HIRATA[1,2], Kumiko GOTO[1,2], Takanori KANAZAWA[1], Kayoko MAEKAWA[2], Kota IWAHORI[2], Hisashi WADA[2] ([1]Shionogi Co., Ltd., [2]Department of Clinical Research in Tumor Immunology of Osaka University)

**ISMS-IP20** Enhanced Anti-tumor Effects of IFN- γ Producing *Bifidobacterium* in Combination with PD-1 Antibody in a Syngeneic Murine Model

○ Satoshi KOBAYASHI[1], Yuji SEKI[1], Koichiro SHIOYA[1], Shiro KATAOKA[1], Li WANG[1], Yuko SHIMATANI[1], Minoru FUJIMORI[2], Shun'ichiro TANIGUCHI[3], Takaaki NAKAMURA[1]
([1]Anaeropharma Science, Inc., [2]Department of Breast Surgery, Tokyo Medical University Ibaraki Medical Center, [3]Department of Comprehensive Cancer Therapy, Shinshu University School of Medicine)

**ISMS-IP21** Genetically Modified Adipocytes, GMAC, for Regenerative Cell Medicine and Gene Therapy

○ Masayuki KURODA[1], Koutaro YOKOTE[2], Yasushi SAITO[3], Masayuki ASO[4] ([1]Center for Advanced Medicine, Chiba University, [2]Department of Clinical Cell Biology and Medicine, Graduate School of Medicine, Chiba University, [3]Superintendent of the hospital bureau, City hall of Chiba, [4]CellGenTech, Inc.)

**ISMS-IP22** Engineered Bacterial Cancer Therapy Using *Bifidobacterium* Secreting Agonistic Anti-4-1BB scFv in the Mouse Model

○ Tomio MATSUMURA[1], Koichiro SHIOYA[1], Yasuyoshi KANARI[1], Yuko SHIMATANI[1], Shiro KATAOKA[1], Shun'ichiro TANIGUCHI[2], Takaaki NAKAMURA[1] ([1]Anaeropharma Science, Inc., [2]Department of Comprehensive Cancer Therapy, Shinshu University School of Medicine)

**ISMS-IP23** Selenoprotein P-neutralizing Antibodies Improve Insulin Secretion in Type 2 Diabetes Mouse Models

○ Xinying YE[1], Yoshiro SAITO[1] ([1]Graduate School of Pharmaceutical Sciences, Tohoku University)

**ISMS-IP24** Targeting Cancer Stromal Fibrin with Antibody-Drug Conjugate in Pancreatic Tumor Mouse Model

○ Kaori HAYASHI[1], Hirobumi FUCHIGAMI[1], Makoto WAKATSUKI[2], Yasuhiro MATSUMURA[1] ([1]Division of Developmental Therapeutics, National Cancer Center Exploratory Oncology Research & Clinical Trial Center, [2]Department of Integrated Bioscience, Graduate School of Frontier Sciences, The University of Tokyo)

**ISMS-IP25** ADC Payload and Linker Chemistry-Dolastatin 10 Analogues and Non-Cleavable Linkers-

○ Michinori AKAIWA[1,2], Tioga MARTIN[2], Brian A. MENDELSOHN[2] ([1]Modality Research Labs. Drug Discovery Research, Astellas Pharma Inc., [2]Agensys Inc.)

**ISMS-IP26** A Novel Strategy for Destabilization of Oncogenic Fusion Protein BCR-ABL to Inhibit Growth of CML

○ Norihito SHIBATA[1], Nobumichi OHOKA[1], Mikihiko NAITO[1] ([1]National Institute of Health Sciences, Division of Molecular Target and Gene Therapy Products)

**ISMS-IP27** Inhibition of Influenza A (H7N9) Virus Replication by the Novel Cap-dependent Endonuclease Inhibitor Baloxavir Marboxil

○ Keiichi TANIGUCHI[1,2], Yoshinori ANDO[1], Haruaki NOBORI[1,2], Shinsuke TOBA[1,2], Takeshi NOSHI[1], Masanori KOBAYASHI[1,3], Makoto KAWAI[1], Ryu YOSHIDA[1], Akihiko SATO[1,2], Takao SHISHIDO[1], Akira NAITO[1], Keita MATSUNO[2,4], Masatoshi OKAMATSU[2], Yoshihiro SAKODA[2,4], Hiroshi KIDA[2,4] ([1]Shionogi & Co., Ltd., [2]Hokkaido University, [3]Gifu University, [4]Global Station for Zoonosis Control, Global Institution for Collaborative Research and Education (GI-CoRE))

**ISMS-IP28** Discovery of TA-8995 (obicetrapib) as a CETP Inhibitor

○ Norimitsu HAYASHI[1], Hitoshi KUBOTA[1], Yoshinori NAKAMURA[1], Yasuo YAMAMOTO[1], Masakatsu SUGAHARA[1], Takanori HIGASHIJIMA[1], Mariko OOI[1], Kozo OKA[1]
([1]Sohyaku. Innovative Research Division, Mitsubishi Tanabe Pharma Corporation)

**ISMS-IP29** Drug Discovery of Novel Aminoglycoside Antibiotics Active Against Multidrug-Resistant Gram-Negative Bacteria

○ Yasunari OTSUKA[1], Eijiro UMEMURA[1], Yoshiaki TAKAHASHI[1], Yukimi TAKAMIYA[1], Teruhisa ISHIBASHI[1], Chigusa HAYASHI[1], Masayuki IGARASHI[1], Masakatsu SHIBASAKI[1]
([1]Institute of Microbial Chemistry (BIKAKEN) )

**ISMS-IP30** Structure Activity Relationship Study of Naturally Occurring Cyclodepsipeptide Destruxins

○ Masahito YOSHIDA[1], Hiroshi SATO[2,3], Gen KONNO[2], Yuna NIWA[4], Mika TOMIDA[4], Hiroshi NAKAGAWA[4], Takayuki DOI[2] ([1]Faculty of Pure and Applied Sciences, University of Tsukuba, [2]Graduate School of Pharmaceutical Sciences, Tohoku University, [3]Mitsubishi Tanabe Pharma Corporation, [4]Department of Applied Biological Chemistry, Chubu University)

**ISMS-IP31** Design Strategy for Potent Dipeptidyl Peptidase IV (DPP-4) Inhibitors by Incorporating Salt Bridge Formation with Lys554

○ Hironobu MAEZAKI[1*], Michiko TAWADA[1], Tohru YAMASHITA[1], Yoshihiro BANNO[1*], Yasufumi MIYAMOTO[1], Yoshio YAMAMOTO[1], Koji IKEDO[1], Takuo KOSAKA[1], Shigetoshi TSUBOTANI[1], Akiyoshi TANI[1], Tomoko ASAKAWA[1], Nobuhiro SUZUKI[1], Satoru OI[1] ([1]Takeda Pharmaceutical Company Limited, [*]Present address: Axcelead Drug Discovery Partners, Inc.)

**ISMS-IP32** Discovery of a Dihydronaphthalene-Based Sphingosine-1-Phosphate (S1P) Receptor Agonist: Ceralifimod (ONO-4641)

○ Haruto KURATA[1], Kensuke KUSUMI[1], Kazuhiro OTSUKI[1], Ryo SUZUKI[1], Masakuni KURONO[1], Takaki KOMIYA[2], Hiroshi HAGIYA[2], Hirotaka MIZUNO[2], Hiroki SHIOYA[2], Takeji ONO[2], Yuka TAKADA[2], Tatsuo MAEDA[2], Norikazu MATSUNAGA[3], Tetsu KONDO[3], Sachiko TOMINAGA[3], Ken-ichi NUNOYA[3], Hidekazu KIYOSHI[4], Masaharu KOMENO[4], Shinji NAKADE[2], Hiromu HABASHITA[1] ([1]Medicinal Chemistry Research Laboratories, [2]Exploratory Research Laboratories, [3]Pharmacokinetic Research Laboratories, [4]Safety Research Laboratories, Ono Pharmaceutical Co., Ltd.)

**ISMS-IP33** Discovery of Clinical Candidate TAK-915, A Highly Potent, Selective, and Brain-Penetrating Phosphodiesterase 2A Inhibitor for the Treatment of Cognitive Disorders

○ Satoshi MIKAMI[1] ([1]Drug Discovery Chemistry Laboratories, Neuroscience Drug Discovery Unit, Research, Takeda Pharmaceutical Company Limited)

**ISMS-IP34** Development of Novel Bicyclic Pyrazoles as Potent and Selective ALK2 (R206H) Inhibitors for the Treatment of Fibrodysplasia Ossificans Progressiva

Hirofumi YAMAMOTO[1], Naoki SAKAI[2], Satoshi OHTE[3], ○ Katsuhiko SEKIMATA[1], Tomohiro SATO[4], Takehisa MATSUMOTO[2], Yoshifumi FUJII[5], Noriko HANDA[5], Hisami WATANABE[2], Chiemi MISHIMA-TSUMAGARI[2], Akiko TANAKA[2], Teruki HONMA[4], Yoshinobu HASHIZUME[6], Shigeyuki YOKOYAMA[5], Hiroshi TOMODA[3], Mikako SHIROUZU[2], Kohei MIYAZONO[7], Hiroo KOYAMA[1] ([1]RIKEN Center for Sustainable Resource Science, Drug Discovery Chemistry Platform Unit, [2]RIKEN Center for Biosystems Dynamics Research, Drug Discovery Structural Biology Platform Unit, [3]Kitasato University, Graduate School of Pharmaceutical Sciences, [4]RIKEN Center for Biosystems Dynamics Research, Drug Discovery Computational Chemistry Platform Unit, [5]RIKEN Systems and Structural Biology Center, Crystallographic Drug Discovery Platform Unit, [6]RIKEN Program for Drug Discovery and Medical Technology Platforms, [7]The University of Tokyo, Graduate School of Medicine, Department of Molecular Pathology)

**ISMS-IP35** Design, Synthesis and Evaluation of 8-(methylamino)-2-oxo-1,2-dihydroquinoline (MAOQ) Derivatives as Novel DNA Gyrase and Topoisomerase IV Inhibitors

○ Fumihito USHIYAMA[1], Hideaki AMADA[1], Takashi YOSHIZUMI[1], Yasuhiro MIHARA[1], Tomoki TAKEUCHI[1], Nozomi YAMAMOTO[1], Junya YAMAGISHI[1], Aiko MASUKO[1], Kiyoko FUJITA[1], Masashi MIMA[1], Koichiro NAKANO[1], Hirotoshi OKUMURA[1], Hiroyuki SUGIYAMA[1], Norikazu OHTAKE[1] ([1]Taisho Pharmaceutical Co., Ltd.)

**ISMS-IP36** Design, Synthesis and Evaluation of Novel Class of Orally Bioavailable eIF4A3-selective Inhibitors

○ Ryo MIZOJIRI[1], Daisuke NAKATA[1], Yoshihiko SATOH[1], Daisuke MORISHITA[1], Misa IWATANI-YOSHIHARA[1], Yohei KOSUGI[1], Mai KOSAKA[1], Junpei TAKEDA[1], Shigekazu SASAKI[1], Kazuaki TAKAMI[1], Masahiro KAMAURA[1], Shinobu SASAKI[1], Ryosuke ARAI[1], Douglas R. CARY[1], Yasuhiro IMAEDA[1] ([1]Takeda Pharmaceutical Company Limited)

**ISMS-IP37** Discovery, SAR and *in vivo* Effects of Novel Natriuretic Peptide Receptor A (NPR-A) agonists

○ Takehiko IWAKI[1], Yuji NAKAMURA[1], Taisaku TANAKA[1], Yasuyuki OGAWA[1], Osamu IWAMOTO[1], Yamato SUZUKI[1], Yoshihiko OKAMURA[1], Yumi KAWASE[1], Akira YAMAKI[1], Makoto IWANAMI[1], Yoshiaki OYAMA[1], Takahiro NAGAYAMA[1] ([1]Daiichi Sankyo CO., LTD.)

**ISMS-IP38** Discovery of Orally Efficacious ROR$\gamma$ Inhibitors Composed of an Isoxazole Scaffold

○ Masayuki KOTOKU[1,3], Takaki MAEBA[1], Shingo FUJIOKA[1], Masahiro YOKOTA[1], Noriyoshi SEKI[1], Keisuke ITO[1], Yoshihiro SUWA[1], Taku IKENOGAMI[1], Kazuyuki HIRATA[1], Yoshiaki KATSUDA[1], Naoki MIYAGAWA[1], Kojo ARITA[1], Kota ASAHINA[1], Masato NOGUCHI[1], Akihiro NOMURA[1], Satoki DOI[1], Tsuyoshi ADACHI[1], Paul CROWE[2], Haiyan TAO[2], Scott THACHER[2], Hiromasa HASHIMOTO[1], Takayoshi SUZUKI[3], Makoto SHIOZAKI[1] ([1]JAPAN TOBACCO INC. Central Pharmaceutical Research Institute, [2]Orphagen Pharmaceuticals, [3]Graduate School of Medical Science, Kyoto Prefectural University of Medicine)

**ISMS-IP39** Discovery of Potent, Orally Available, and Brain-Penetrating Receptor Interacting Protein 1 (RIP1) Kinase Inhibitors: Analysis of Structure − Kinetic Relationships

○ Masato YOSHIKAWA[1] ([1]Neuroscience Drug Discovery Unit, Research, Takeda Pharmaceutical Company Limited)

**ISMS-IP40** Estimating Efflux Transporter-mediated Disposition Using Transporter Gene Knockout Rats

○ Taiji MIYAKE[1] ([1]Discovery ADMET Dept., Research Div., Chugai Pharmaceutical Co., Ltd.)

**ISMS-IP41** Prediction of Human Distribution Volumes of Compounds in Various Elimination Phases Using Physiologically Based PK Modeling and Experimental PK in Animals

○ Hidetoshi SHIMIZU[1], Kosuke YOSHIDA[1], Tomohisa NAKADA[1], Koki KOJIMA[1], Akihito OGASAWARA[1], Yoshinobu NAKAMARU[1], Hiroshi YAMAZAKI[2] ([1]Mitsubishi Tanabe Pharma Corporation, [2]Showa Pharmaceutical University)

**ISMS-IP42** Supersaturated Transdermal Formulation Designed by Co-amorphous System

○ Yuya HIRAKAWA[1,2], Hiroshi UEDA[1], Tetsuya MIYANO[1], Noriho KAMIYA[2], Masahiro GOTO[2] ([1]Research Laboratory for Development, Shionogi & Co., Ltd., [2]Department of Applied Chemistry, Kyushu University)

**ISMS-IP43** Kilogram-Scale Synthesis of Esomeprazole and Related Proton Pump Inhibitors through Iron-Catalyzed Enantioselective Sulfoxidation

○ Shigenobu NISHIGUCHI[1], Takuhiro IZUMI[1], Takayoshi KOUNO[2], Junpei SUKEGAWA[1], Laurean ILIES[3,4], Eiichi NAKAMURA[4] ([1]Towa Pharmaceutical Co., Ltd., [2]Daichikasei Co., Ltd., [3]RIKEN, [4]Tokyo University)