

新学術領域研究「化学コミュニケーションのフロンティア (FY2017-2021)」

成果発表リスト A03 (計画研究, Project Groups) FY2017~2021

1. 菊地和也 (大阪大学大学院工学研究科・教授)

KIKUCHI, Kazuya (Professor, Osaka University)

【原著論文, original journal】

- 1) Reja, S. I., Hori, Y., Kamikawa, T., Yamasaki, K., Nishiura, M., Bull, S. D., *Kikuchi, K. An "OFF-ON-OFF" fluorescence protein-labeling probe for real-time visualization of the degradation of short-lived proteins in cellular systems. *Chem. Sci.*, 13, 1419-1427, doi: 10.1039/D1SC06274C, 2022.
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- 3) Vicente, M., Salgado-Almario, J., Collins, M. M., Martínez-Sielva, A., Minoshima, M., Kikuchi, K., Domingo, B., *Llopis, J. Cardioluminescence in transgenic zebrafish larvae: A calcium imaging tool to study drug effects and pathological modeling. *Biomedicines*, 9, 1294, doi: 10.3390/biomedicines9101294, 2021.
- 4) Konishi, Y., Okunishi, A., Sugihara, F., Nakamura, T., Akazawa, K., Minoshima, M., *Kikuchi, K. Development of Off-On Switching ¹⁹F MRI Probes for Cathepsin K Activity Detection. *Bull. Chem. Soc. Jpn.*, 94, 1690-1694, doi: 10.1246/bcsj.20210099, 2021.
- 5) Kowada, T., Arai, K., Yoshimura, A., Matsui, T., *Kikuchi, K., *Mizukami, S. Optical Manipulation of Subcellular Protein Translocation Using a Photoactivatable Covalent Labeling System. *Angew. Chem. Int. Ed.*, 60, 11378-11383, doi: 10.1002/anie.202016684, 2021.
- 6) Hori, Y., Nishiura, M., Tao, T., Baba, R., Bull, S. D., *Kikuchi, K. Fluorogenic probes for detecting deacylase and demethylase activity towards post-translationally-modified lysine residues. *Chem. Sci.*, 12, 2498-2503, doi: 10.1039/D0SC06551J, 2021.
- 7) Kumar, N., Hori, Y., Nishiura, M., *Kikuchi, K. Rapid No-wash Labeling of PYP-tag Proteins with Reactive Fluorogenic Ligands Affords Stable Fluorescent Protein Conjugates for Long-Term Cell Imaging Studies. *Chem. Sci.* 11, 3694-3701, doi: 10.1039/D0SC00499E, 2020.
- 8) Torii, K., Hori, Y., Watabe, K., *Kikuchi, K. Development of Photoswitchable Fluorescent Molecules Using Arylazopyrazole. *Bull. Chem. Soc. Jpn.* 93, 821-824, doi: 10.1246/bcsj.20200077, 2020.
- 9) Hashimoto, R., Minoshima, M., Kikuta, J., Yari, S., Bull, S.D., Ishii, M., *Kikuchi, K. An Acid Activatable Fluorescence Probe for Imaging Osteocytic Bone Resorption Activity in Deep Bone Cavities. *Angew. Chem. Int. Ed.* 59, 20996-21000, doi: 10.1002/anie.202006388, 2020.
- 10) Imoto, T., Minoshima, M., Yokoyama, T., Emery, B.P., Bull, S.D., Bito, H., *Kikuchi, K. A Photoactivatable Antagonist for Controlling CREB Dependent Gene Expression. *ACS Cent. Sci.* 6, 1813-1818, doi: 10.1021/acscentsci.0c00736, 2020. [Selected as a cover feature.]
- 11) Tomczyk, M.M., *Boncel, S., Herman, A., Krawczyk, T., Jakóbk-Kolon, A., Pawlyta, M., Krywiecki, M., Chrobak, A., Minoshima, M., Sugihara, F., Kikuchi, K., *Kuźnik, N. Oxygen Functional Groups on MWCNT Surface as Critical Factor Boosting T₂ Relaxation Rate of Water Protons: Towards Improved CNT-Based Contrast Agents. *Int. J. Nanomed.* 15, 7433-7450, doi: 10.2147/IJN.S257230, 2020.
- 12) *Imamura, H., Sakamoto, S., Yoshida, T., Matsui, Y., Penuela, S., Laird, D.W., Mizukami, S., Kikuchi, K., Kakizuka A. Single-cell Dynamics of Pannexin-1-facilitated Programmed ATP Loss during Apoptosis. *eLife*, 9, e61960, doi: 10.7554/eLife.61960, 2020.
- 13) Wyskocka-Gajda, M., Przepis, L., Olesiejuk, M., Krawczyk, T., Kuźnik, A., Nawara, K., Minoshima, M., Sugihara, F., Kikuchi, K., *Kuźnik, N. A Step towards Gadolinium-free Bioresponsive MRI Contrast Agent, *Eur. J. Med. Chem.* 211, 113086, doi: 10.1016/j.ejmech.2020.113086, 2020.
- 14) Hori, Y., Nishiura, M., Tao, T., Baba, R., Bull, S.D. *Kikuchi, K. Fluorogenic Probes for Detecting Deacylase and Demethylase Activity towards Post-translationally-modified Lysine Residues, *Chem. Sci.* 12, 2498-2503,

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- 15) Kowada, T., Arai, K., Yoshimura, A., Matsui, T., *Kikuchi, K., *Mizukami, S. Optical Manipulation of Subcellular Protein Translocation Using a Photoactivatable Covalent Labeling System, *Angew. Chem. Int. Ed.* 60, 11378-11383, doi: 10.1002/anie.202016684, 2021.
- 16) Gao, J., Hori, Y., Takeuchi, O., *Kikuchi, K. "Live-Cell Imaging of Protein Degradation Utilizing Designed Protein-Tag Mutant and Fluorescent Probe with Turn-Off Switch" *Bioconjugate Chem.* 31, 577-583, doi: 10.1021/acs.bioconjchem.9b00696, 2020.
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- 18) Gao, J., Hori, Y., Nishiura, M., Bordy, M., Hasserodt, J., *Kikuchi, K., "Engineered Protein-tag for Rapid Live-cell Fluorogenic Visualization of Proteins by Anionic Probes" *Chem Lett.*, 49, 232-235, 2020.
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- 22) Minoshima, M., Kikuta, J., Omori, Y., Seno, S., Suehara, R., Maeda, H., Matsuda, H., Ishii, M., *Kikuchi, K. "In vivo Multicolor Imaging with Fluorescent Probes Revealed the Dynamics and Function of Osteoclast Proton Pumps" *ACS Cent. Sci.*, 5, 1059-1066, 2019.
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- 31) Sato, R., Kozuka, J., Ueda, M., Mishima, R., Kumagai, Y., Yoshimura, A., Minoshima, M., Mizukami, S.,

*Kikuchi, K., “Intracellular Protein-Labeling Probes for Multicolor Single-Molecule Imaging of Immune Receptor-Adaptor Molecular Dynamics” *J. Am. Chem. Soc.* 139, 17397-17404, 2017.

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【解説・総説, review】

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- 2) Reja, S. I., Minoshima, M., Hori, Y., *Kikuchi, K. Near-infrared fluorescent probes: a next-generation tool for protein-labeling applications. *Chem. Sci.*, 12, 3437-3447, doi: 10.1039/D0SC04792A, 2021.
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- 5) Reja, S.I., Minoshima, M., Hori, Y., *Kikuchi, K., “Development of an Effective Protein-labeling System Based on Smart Fluorogenic Probes” *J. Biol. Inorg. Chem.*, 24, 443-455, 2019.
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- 7) Kumar, N., Hori, Y., *Kikuchi, K., “Live-Cell Imaging of DNA Methylation Based on Synthetic-Molecule/Protein Hybrid Probe” *Chem. Rec.*, 18, 1672-1680, 2018.

【著書】

- 1) 蓑島維文, 菊地和也. 先端の分析法第 2 版 (原理編第 3 章プローブ, MRI プローブ), エヌティーエス出版, 2022. (2022 年 1 月発刊)
- 2) 蓑島維文, 菊地和也. 「第 5 章 2 MRI プローブ」核酸科学ハンドブック, 杉本直己 (編), 日本核酸化学会 (監修), 講談社サイエンティフィック, 156-164, 2020.
- 3) 蓑島維文, 菊地和也. 「機能性セレンテラジンをを用いた発光検出」発光イメージング実験ガイド, 実験医学別冊, 永井健治・小澤岳昌編, 羊土社, 71-78, 2019.

【招待講演・基調講演】

国際 :

- 1) *Kikuchi, K. Nano-particle based ¹⁹F MRI contrast agent with tunable chemical switches. (#249 Innovative New Chemistry for MRI Contrast), PACIFICHEM2021, Hawaii, USA, Dec. 2021. (招待講演)
- 2) Kikuchi, K. in vivo Imaging Probes to Clarify Cellular and Molecular Functions. RSC Tokyo International Conferences 2020. Tokyo, Japan, Dec. 2020. (plenary lecture) (招待講演)
- 3) Kikuchi, K. “New Biological Findings which were Revealed by Designed Fluorescent Probes” Chemical Biology & Physiology Conference 2019, Portland, OR, USA, December 12-15, 2019 (招待講演)
- 4) Kikuchi, K. “In vivo Multicolor Imaging with Fluorescent Probes Revealed Dynamics and Function of Osteoclast Proton Pumps” 16th International, Methods & Applications of Fluorescence (Roger Y Tsien Memorial Symposium), La Jolla, CA USA, August 20-24, 2019 (招待講演)
- 5) Kikuchi, K. “in vivo Chemical Probes for MRI and Fluorescence Imaging” (Keynote lecture) ICBIC-19, International Conference on Biological Inorganic Chemistry, Interlaken, Switzerland, August 11-16, 2019 (招待講演)
- 6) Kikuchi, K. “Development of Multifunctional ¹⁹F MRI Contrast Agents Based on Fluorine-encapsulated Silica Nanoparticle” The Future of Molecular MR: A Cellular and Molecular Imaging Workshop, St. John’s, NF Canada, July 14-17, 2019 (招待講演)

- 7) Kikuchi, K. “In Vivo Chemical Probes for MRI and Fluorescence Imaging”, 9th Asian Biological Inorganic Chemistry Conference (AsBIC9), 9-14 December 2018, Singapore. (Plenary Lecture)
- 8) Kikuchi, K. “New Biological Findings Which Were Revealed by Designed Chemical Probes”, A3 Meeting for Chemical Biology, 31 October-3 November, 2018, Jeju, Korea.
- 9) Kikuchi, K. “Development of Multifunctional ¹⁹F MRI Contrast Agents Based on Fluorine-encapsulated Silica Nanoparticle”, Imaging in 2020, 23-27 September, 2018, Wyoming, USA.
- 10) Kikuchi, K. “New Biological Findings Which Were Clarified by Designed Chemical Probes” Ruhr-Universitaet Bochum, Japan Science Days, 5-7 July, 2018, Bochum, Germany.
- 11) Kikuchi, K. “In Vivo Imaging Probes with Tunable Chemical Switches” 6th International Conference on Molecular Sensing and Molecular Logic Gates (MSMLG2018), 3-6 June, 2018, Dalian, China.
- 12) Kikuchi, K. “New Biological Findings Which Were Clarified by Designed Chemical Probes” 2018 Queenstown Molecular Biology Meetings in Shanghai, 22-23 March, 2018, Shanghai, China.
- 13) Kikuchi, K. “Tunable In Vivo Imaging Probes with Functional Metal Complex Switches” 14th International Conference on Applied Bioinorganic Chemistry (ISABC14), 7-10 June, 2017, Toulouse, France. (基調講演)

国内：

- 1) 菊地和也. 化学プローブによって明らかになった生命現象. 日本分析化学会第68年会 (日本分析化学会主催), 千葉, 9月, 2019. (招待講演)
- 2) 菊地和也. イメージングプローブのデザイン・合成によるケミカルバイオロジー研究. 第19回日本蛋白質科学会年会 第71回日本細胞生物学会大会 合同年次学会 (日本蛋白質科学会、日本細胞生物学会主催), 神戸, 6月, 2019. (招待講演)
- 3) 菊地和也. 「GLUT4の糖鎖機能を可視化する局在痕跡イメージングプローブ」日本農芸化学会2018年度大会. 名古屋, 3月, 2018.

【特許等の出願状況】

- 1) 薫島維文, 橋本 龍, 菊地和也. ケージド化合物から化合物を放出させる方法. 国立大学法人大阪大学. 特願 2021-022014, 出願日: 令和3年2月15日. 国内.

【報道記事】

【受賞・表彰】

【アウトリーチ活動】

- 1) 高校生向けに出張授業を行い、関連領域の紹介を行った (宮崎大宮高校, 2018年3月13日)。

2. 榊原康文 (慶應義塾大学理工学部・教授)
SAKAKIBARA, Yasubumi (Professor, Keio University)

【原著論文, originai journal】

- 1) Akiyama, M., *Sakakibara, Y. Informative RNA base embedding for RNA structural alignment and clustering by deep representation learning. *NAR Genom. Bioinform.* In press, 2022.
- 2) Yoshimura, Y., Hamada, A., Augey, Y., Akiyama, M., *Sakakibara, Y. Genomic style: yet another deep-learning approach to characterize bacterial genome sequences. *Bioinformatics Advances* 1(1), vbab039, doi.org/10.1093/bioadv/vbab039, 2021.
- 3) Watanabe, N., Ohnuki, Y., *Sakakibara, Y. Deep learning integration of molecular and interactome data for protein-compound interaction prediction. *J Cheminform.* 13(1), 36, doi: 10.1186/s13321-021-00513-3, 2021.

- 4) Liang, K.C., *[Sakakibara, Y.](#) MetaVelvet-DL: a MetaVelvet deep learning extension for de novo metagenome assembly. *BMC Bioinform.* 22(6), 427, doi.org/10.1186/s12859-020-03737-6, 2021.
- 5) Jayakumar, V., Nishimura, O., Kadota, M., Hirose, N., Sano, H., Murakawa, Y., Yamamoto, Y., Nakaya, M., Tsukiyama, T., Seita, Y., Nakamura, S., Kawai, J., Sasaki, E., Ema, M., Kuraku, S., *Kawaji, H., *[Sakakibara, Y.](#) Chromosomal-scale de novo genome assemblies of Cynomolgus Macaque and Common Marmoset. *Sci Data.* 8(1), 159, doi: 10.1038/s41597-021-00935-6, 2021.
- 6) [Sato, K.](#), Kato, Y. Prediction of RNA secondary structure including pseudoknots for long sequences, *Brief. Bioinform.* 23, doi: 10.1093/bib/bbab395, 2022. [Press release]
- 7) Kashiwagi, S., *[Sato, K.](#), [Sakakibara, Y.](#) A max-margin model for predicting residue-base contacts in protein-RNA interactions. *Life.* 11(11):1135, doi: 10.3390/life11111135, 2021.
- 8) [Saito, Y.](#), Oikawa, M., Sato, Nakazawa, T., H., Ito, T., Kameda, T., *Tsuda, K., *Umetsu, M. Machine-learning-guided library design cycle for directed evolution of enzymes: the effects of training data composition on sequence space exploration. *ACS Catalysis*, 11(23):14615-14624, doi: 10.1021/acscatal.1c03753, 2021. Selected as Cover Art.
- 9) Suzuki, G., [Saito, Y.](#), Seki, M., Evans-Yamamoto, D., Negishi, M., Kakoi, K., Kawai, H., Landry, C.R., *Yachie, N., *Mitsuyama, T. Machine learning approach for discrimination of genotypes based on bright-field cellular images. *NPJ Syst. Biol. Appl.* 7(1):31, doi: 10.1038/s41540-021-00190-w, 2021.
- 10) Yamaguchi, H., *[Saito, Y.](#) Evotuning protocols for Transformer-based variant effect prediction on multi-domain proteins. *Brief. Bioinformatics*, 22(6):bbab234, doi: 10.1093/bib/bbab234, 2021.
- 11) Tajima, N., Kumagai, T., [Saito, Y.](#), *Kameda, T. Comparative analysis of the relationship between translation efficiency and sequence features of endogenous proteins in multiple organisms. *Genomics*, 113(4):2675-2682, doi: 10.1016/j.ygeno.2021.05.037, 2021.
- 12) Irumagawa, S., Kobayashi, K., [Saito, Y.](#), Miyata, T., Umetsu, M., Kameda, T., *Arai, R. Rational thermostabilisation of four-helix bundle dimeric de novo proteins. *Sci. Rep.*, 11(1):7526, doi: 10.1038/s41598-021-86952-2, 2021.
- 13) *[Sato, K.](#), Akiyama, M., [Sakakibara, Y.](#) RNA secondary structure prediction using deep learning with thermodynamic integration. *Nat. Commun.* 12, 941, doi: 10.1038/s41467-021-21194-4, 2021. [press release]
- 14) Miyazaki, Y., Oda, T., Inagaki, Y., Kushige, H., [Saito, Y.](#), Mori, N., Takayama, Y., Kumagai, Y., Mitsuyama, T., *Kida, S.Y. Adipose-derived mesenchymal stem cells differentiate into heterogeneous cancer-associated fibroblasts in a stroma-rich xenograft model. *Sci. Rep.* 11(1):4690, doi: 10.1038/s41598-021-84058-3, 2021.
- 15) Jayakumar, V., Ishii, H., Seki, M., Kumita, W., Inoue, T., Hase, S., [Sato, K.](#), Okano, H., Sasaki, E., *[Sakakibara, Y.](#) An improved de novo genome assembly of the common marmoset genome yields improved contiguity and increased mapping rates of sequence data. *BMC Genomics* 21, 243, doi: 10.1186/s12864-020-6657-2, 2020.
- 16) Kurumida, Y., [Saito, Y.](#), *Kameda, T. Predicting antibody affinity changes upon mutations by combining multiple predictors. *Sci. Rep.* 10(1):19533, doi: 10.1038/s41598-020-76369-8, 2020.
- 17) Lee, J.H., [Saito, Y.](#), Park, S.J., * Nakai, K. Existence and possible roles of independent non-CpG methylation in the mammalian brain. *DNA Research*, 27(4):dsaa020, doi: 10.1093/dnares/dsaa020, 2020.
- 18) Nguyen, T. D., [Saito, Y.](#), *Kameda, T. CodonAdjust: a software for in silico design of a mutagenesis library. *Protein Eng. Des. Sel.* 32(11):503-511, doi: 10.1093/protein/gzaa013, 2019.
- 19) Liang KC, *[Sakakibara, Y.](#) MetaVelvet-DL: a MetaVelvet deep learning extension for de novo metagenomics assembly. *BMC Bioinformatics*, in press, 2020.
- 20) Nakato, R., *Wada, Y., Nakaki, R., Nagae, G., Katou, Y., Tsutsumi, S., Nakajima, N. Fukuhara, H., Iguchi, A., Kohro, T., Kanki, Y., [Saito, Y.](#), Kobayashi, M., Izumi-Taguchi, A., Osato, N., Tatsuno, K., Kamio, A., Hayashi-Takanaka, Y., Wada, H., Ohta, S., Aikawa, M., Nakajima, H., Nakamura, M., McGee, R. C., Heppner, K. W., Kawakatsu, T., Genno, M., Yanase, H., Kume, H., Senbonmatsu, T., Homma, Y., Nishimura, S., Mitsuyama, T., Aburatani, H., * Kimura, H., * Shirahige, K. Comprehensive epigenome characterization reveals diverse transcriptional regulation across human vascular endothelial cells. *Epigenetics Chromatin*, 12:77, 2019.
- 21) [Saito, Y.](#), Kitagawa, W., Kumagai, T., Tajima, N., Nishimiya, Y., Tamano, K., Yasutake, Y., * Tamura, T., *Kameda, T. Developing a codon optimization method for improved expression of recombinant proteins in actinobacteria. *Sci. Rep.* 9(1):8338, 2019. [press release]

- 22) Hirohara, M., [Saito, Y.](#), Koda, Y., [Sato, K.](#), [Sakakibara, Y.](#) Convolutional neural network based on SMILES representation of compounds for detecting chemical motif. *BMC Bioinformatics*, 19, 526, 2018.
- 23) Aoto, Y., Okumura, K., Hachiya, T., Hase, S., Wakabayashi, Y., Ishikawa, F., [Sakakibara, Y.](#) Time-Series Analysis of Tumorigenesis in a Murine Skin Carcinogenesis Model. *Sci. Rep.* 8, 12994, 2018.
- 24) Aoki, G., [Sakakibara, Y.](#) Convolutional neural networks for classification of alignments of non-coding RNA sequences. *Bioinformatics*, 34, i237-i 244, 2018.
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- 27) Aoto, Y., Hachiya, T., Okumura, K., Hase, S., [Sato, K.](#), Wakabayashi, Y., [Sakakibara, Y.](#) DEclust: A statistical approach for obtaining differential expression profiles of multiple Conditions. *PLoS One*, 12, e0188285, 2017.

【解説・総説, review】

- 1) [佐藤健吾](#). MXfold2: 深層学習にもとづく RNA の高精度な二次構造予測プログラム. *バイオサイエンスとインダストリー*, 79(6):482-483, 2021.
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【著書】

【招待講演・基調講演】

国内：

- 1) [榎原康文](#). 医療と AI(人工知能)のマッチング. 第 94 回日本内分泌学会学術総会. オンライン開催. 4 月, 2021. (特別講演)
- 2) [齋藤 裕](#). タンパク質工学における機械学習の利用. 公益社団法人新化学技術推進協会ライフサイエンス技術部会反応分科会 技術セミナー「AI の基礎と応用：タンパク質の機能変化を題材に」. オンライン開催. 12 月, 2020.
- 3) [榎原康文](#). 慶應大学における医療への AI 活用の現状と動向について. 公益社団法人日本技術士会神奈川県支部 第 80 回 CPD 講座「ここまで進んだ医療・生命科学への AI の活用」. 波止場会館, 神奈川県, 5 月, 2019. (招待講演)
- 4) [齋藤 裕](#). 人工知能と実験の融合による生物工学研究. 公益社団法人日本技術士会神奈川県支部 第 80 回 CPD 講座「ここまで進んだ医療・生命科学への AI の活用」. 波止場会館, 神奈川県, 5 月, 2019. (招待講演)

- 5) 佐藤健吾. 「機械学習を用いた RNA 二次構造予測」日本バイオインフォマティクス学会九州地域部会セミナー. 九州大学西新プラザ, 12 月, 2018.

【特許等の出願状況】

【報道記事】

- 1) 「慶大と阪大、より複雑で長い RNA の二次構造を高速に予測可能に」, 日本経済新聞, 2021. 10. 6.
- 2) 「慶大と阪大、より複雑で長い RNA の二次構造を高速に予測可能に」, 日経バイオテク, 2021. 10. 6.
- 3) 「慶大など、RNA 二次構造を高速・高精度に予測 計算モデルを変更」, 日刊工業新聞, 2021. 10. 6.
- 4) 「人工知能で酵素を自動設計—様々な機能性タンパク質開発の加速に期待—」, 東北大学 HP, 理化学研究所 HP
https://www.tohoku.ac.jp/japanese/newimg/pressimg/tohokuuniv-press20211202_01web_ai.pdf
https://www.riken.jp/press/2021/20211202_4/index.html
- 5) 「東北大と理研、タンパク質の機能設計を人工知能によって効率化する手法を開発」, 日本経済新聞電子版
https://www.nikkei.com/article/DGXLRS622897_S1A201C2000000/
- 6) 「RNA 二次構造予測で世界最高精度を達成」, 慶應義塾大学 HP
URL: <https://www.keio.ac.jp/ja/press-releases/2021/2/12/28-78076/>
- 7) 「産総研グループ 微生物の蛋白質量を向上 遺伝子配列設計技術で」, 薬事日報 (朝刊 17 面, 7/17, 2019)
- 8) 「微生物のタンパク質生産量向上 産総研 遺伝子配列設計技術開発」, 科学新聞 (朝刊 1 面, 6/28, 2019)
- 9) 「産総研 微生物利用たんぱく質 生産量向上へ新手法」, 化学工業日報 (朝刊 3 面, 6/14, 2019)

【受賞・表彰】

- 1) Best Talk Award (First Prize). Hideki Yamaguchi, Yutaka Saito. Evotuning protocols for Transformer-based variant effect prediction on multi-domain proteins. The 29th International Conference on Intelligent Systems for Molecular Biology and The 20th European Conference on Computational Biology (ISMB / ECCB 2021). Online, Jul 25 - Jul 30, 2021.
- 2) ポスター賞. Hideki Yamaguchi, Yutaka Saito. Accurate prediction of variant effects by efficient incorporation of evolutionary information into Transformer-based deep learning. 第 21 回 日本蛋白質科学会年会. 6/16 - 6/18, 2021. オンライン開催.
- 3) 齋藤 裕. ポスター賞, 「深層強化学習を用いた二次構造に基づく RNA 配列の設計」, 第 9 回生命医薬情報学連合大会 (IIBMP2020), 2020 年 9 月 3 日.
- 4) 優秀ポスター発表賞. Hideki Yamaguchi, Yutaka Saito. Evolutionary training protocols for deep representation learning of multi-domain proteins. 日本バイオインフォマティクス学会 2020 年年会, 第 9 回 生命医薬情報学連合大会 (IIBMP 2020). 9/1 - 9/3, 2020. オンライン開催.
- 5) 優秀ポスター発表賞. Shuzo Fukunaga, Hideki Yamaguchi, Yutaka Saito. 深層表現学習によるタンパク質の指向性進化と自然進化の関連解析. 日本バイオインフォマティクス学会 2020 年年会, 第 9 回 生命医薬情報学連合大会 (IIBMP 2020). 9/1 - 9/3, 2020. オンライン開催.
- 6) Best Activator Award. Shuzo Fukunaga, Hideki Yamaguchi, Yutaka Saito. 深層表現学習によるタンパク質の指向性進化と自然進化の関連解析. 生命情報科学若手の会 第 12 回研究会. 8/27 - 8/28, 2020. オンライン開催.

【アウトリーチ活動】

3. Charles Boone (理化学研究所環境資源科学研究センター・チームリーダー)
Charles M. Boone (Team Leader, RIKEN Center for Sustainable Research Science)

【原著論文, original journal】

- 1) Ohnuki, S., Ogawa, I., Itto-Nakama, K., Lu, F., Ranjan, A., Kabbage, M., Gebre, AA., Yamashita, M., Li, S.C., Yashiroda, Y., Yoshida, S., Usui, T., Piotrowski, JS., Andrews, BJ., Boone, C., Brown, GW., Ralph, J., *Ohya, Y. High-throughput platform for yeast morphological profiling predicts the targets of bioactive compounds. *NPJ Syst. Biol. Appl.* 8, 3, doi: 10.1038/s41540-022-00212-1, 2022.
- 2) Kubo, K., Itto-Nakama, K., Ohnuki, S., Yashiroda, Y., Li, S.C., Kimura, H., Kawamura, Y., Shimamoto, Y., Tominaga, KI., Yamanaka, D., Adachi, Y., Takashima, S., Noda, Y., Boone, C., *Ohya, Y. Jerveratrum-type steroidal alkaloids inhibit β -1,6-glucan biosynthesis in fungal cell walls. *Microbiol. Spectr.* 10, e0087321, doi: 10.1128/spectrum.00873-21, 2022.
- 3) Fu, C., Zhang, X., Veri, AO., Iyer, KR., Lash, E., Xue, A., Yan, H., Revie, NM., Wong, C., Lin, ZY., Polvi, EJ., Liston, SD., VanderSluis, B., Hou, J., Yashiroda, Y., Gingras, AC., Boone, C., O'Meara, TR., O'Meara, MJ., Noble, S., Robbins, N., *Myers, CL., *Cowen, LE. Leveraging machine learning essentiality predictions and chemogenomic interactions to identify antifungal targets. *Nat. Commun.* 12, 6497, doi: 10.1038/s41467-021-26850-3, 2021.
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- 10) Kintaka, R., Makaanae, K., Namba, S., Kato, H., Kito, K., K., Ohnuki, S., Ohya, Y., Andrews, B. J., Boone, C., *Moriya, H. Genetic profiling of protein burden and nuclear export overload. *Elife* 9, e54080, doi: 10.7554/eLife.54080, 2020.
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【解説・総説, review】

- 1) *Kuzmin, E., Taylor, JS., Boone, C. Retention of duplicated genes in evolution. *Trends Genet.* 38, 59, doi: 10.1016/j.tig.2021.06.016, 2022.
- 2) Usaj, MM, Yeung, CHL., Friesen, H., Boone, C., *Andrews, BJ. Single-cell image analysis to explore cell-to-cell heterogeneity in isogenic populations. *Cell Syst.* 12, 608, doi: 10.1016/j.cels.2021.05.010, 2021.
- 3) *Yashiroda, Y., Yoshida, Y. Intraspecies cell-cell communication in yeast. *FEMS Yeast Res.* 19, foz071, 2019.

【著書】

- 1) 八代田陽子, 吉田稔. 第9章酵母ケミカルゲノミクスを用いた化合物作用機序解明のための大規模高速解析法. 酵母菌・麹菌・乳酸菌の産業応用展開 (五味勝也, 阿部敬悦監修), pp. 79-86, 2018.

【招待講演・基調講演】

国際：

- 1) Boone Charles. Institute of Molecular Genetics and Cell Biology, Ulm University, Germany, July. 2021. (invited talk)
- 2) Boone Charles. CIFAR, Fungal Kingdom, July 2021. (invited talk)
- 3) Boone Charles. CIFAR, Fungal Kingdom, Nov. 2021. (invited talk)
- 4) Boone Charles. Genetic Network Analysis of the NGLY1 Pathway. International Symposium on Glycolipidology. Wako, Jan. 2020. (招待講演)
- 5) Yashiroda, Y. Yeast Chemical Genomic Approach for Target Identification. Asian Chemical Biology Initiative (ACBI) 2019 Yangon Meeting, Yangon, Myanmar, January, 2019.
- 6) Boone Charles. Mapping Genetic Networks on a Global Scale. From Genetic Networks to a Cellular Wiring Diagram, Tokyo, Japan, April, 2017.

国内：

- 1) 八代田陽子. 酵母ケミカルゲノミクス法による化合物の標的同定. 第19回日本蛋白質科学会年会 第71回日本細胞生物学会大会合同年次大会共催シンポジウム「化学コミュニケーションのフロンティア」, 神戸, 6月, 2019. (招待講演)
- 2) Boone Charles. 「Mapping Chemical-Genetic Interactions to Link Bioactive Compounds to Cellular Targets」 「化学コミュニケーションのフロンティア」第2回公開シンポジウム. 京都, 2月, 2018.
- 3) 八代田陽子. 「アミノ酸取り込みを調節する酵母細胞間相互作用」 ライフイベントを紡ぐ栄養環境への適応機構. 2017年度生命科学系学会合同年次大会ワークショップ. 神戸, 12月, 2017.

- 4) 八代田陽子. 「脂肪酸化合物を介した酵母細胞間のコミュニケーション」 ファイトバイオーム：植物化学物質による生物間コミュニケーションへの誘い. 第 54 回植物化学シンポジウム. 東京, 11 月, 2017.
- 5) 八代田陽子. 「窒素代謝を変えるコミュニケーション-脂肪酸をつかった分裂酵母の種の生存戦略-」微生物の「声」が聴きたくて...単細胞生物のコミュニケーションスキル. 第 69 回日本生物工学会シンポジウム. 東京, 9 月, 2017.

【特許等の出願状況】

【報道記事】

- 1) 「Drugs Made in Nature: Donnelly Researchers Team up with Japanese Scientists to Mine Microbes for New Therapeutics」, Donnelly Centre News. URL: <https://www.thedonnellycentre.utoronto.ca/node/1341>
- 2) "A smarter way to screen molecular libraries" RIKEN Research (October 6, 2017) <http://www.riken.jp/en/research/rikenresearch/highlights/20170023/>
- 3) 「化合物の標的機能を決定するツールを開発－酵母の化学遺伝学アプローチで化合物の標的予測／同定が迅速に－」、理化学研究所、プレスリリース (July 25, 2017) http://www.riken.jp/pr/press/2017/20170725_1
- 4) "Scientists Enlist Baker's Yeast to Find New Medicines", University of Toronto, News (July 17, 2017) <http://www.thedonnellycentre.utoronto.ca/news/scientists-enlist-baker's-yeast-find-new-medicines>

【受賞・表彰】

- 1) RIKEN Researcher Incentive Award in FY2017, “Target Identification Using an Integrated Chemical Genomic Approach”, Li Sheena, March 2018

【アウトリーチ活動】

- 1) 理化学研究所主催の一般公開（埼玉県和光市, 2019 年 4 月 21 日）の進路相談会において、小・中・大学生（3 名）に対する相談員を務めた。（八代田陽子）
- 2) 東京大学女子卒業生同窓会さつき会の会報「さつき」第 58 号（2019 年 5 月発行、理系研究職特集）にて研究職・研究内容について執筆した。（八代田陽子）
- 3) 理化学研究所主催の見学プログラム（埼玉県和光市, 2019 年 6 月 14 日）において、一般の方 15 名に対して、創薬研究の紹介を行った。（八代田陽子）
- 4) 理化学研究所主催の高校生見学プログラム（埼玉県和光市, 2019 年 11 月 15 日）において、埼玉県立和光国際高等学校 3 年生 27 名に対して、創薬研究の紹介を行った。（八代田陽子）
- 5) 理化学研究所主催の高校生見学プログラム（埼玉県和光市, 2019 年 12 月 11 日）において、武蔵越生高等学校（埼玉県）の生徒 15 名に対して、創薬研究の紹介を行った。（八代田陽子）
- 6) 第 41 回日本分子生物学会年会（パシフィコ横浜, 2018 年 11 月 28 日～30 日）において、【化学コミュニ】後援によるワークショップ『生物間の化学コミュニケーション ～化合物を通じた生命の生き残り戦略～(Chemical communication, a survival strategy of living organisms)』を開催した。（八代田陽子）
- 7) 理化学研究所主催の高校生見学プログラム（埼玉県和光市, 2018 年 10 月 3 日）において、岩手県立一関第一高等学校（2 年生 40 名、引率 2 名）に対して、創薬研究の紹介を行った。（八代田陽子）

4. 長田裕之 (理化学研究所環境資源科学研究センター・グループディレクター)

OSADA Hiroyuki (Group Director, RIKEN Center for Sustainable Research Science Chemical Biology Research Group)

【原著論文, original journal】

- 1) Yoshioka, H., Kawamura, T., Muroi, M., Kondoh, Y., Honda, K., Kawatani, M., Aono, H., Waldmann, H., Watanabe, N., *Osada, H. Identification of a small molecule that enhances ferroptosis via inhibition of ferroptosis suppressor protein 1 (FSP1). *ACS Chem. Biol.* in press. [Press release]
- 2) Jang, J.P., Jang, M., Nogawa, T., Takahashi, S., Osada, H., Ahn, J.S., Ko, S.K., *Jang, J.H. RK-270D and E, oxindole derivatives from *Streptomyces* sp. with anti-angiogenic activity. *J. Microbiol. Biotechnol.* doi: 10.4014/jmb.2110.10039, 2022.
- 3) Liu, H., Panjkar, S., Sheng, X., Futamura, Y., Zhang, C., Shao, N., Osada, H., *Zou, H. β -Methyltryptamine provoking the crucial role of strictosidine synthase Tyr151-OH for its stereoselective plectrolytic reactions to tryptoline-type alkaloids. *ACS Chem. Biol.* 17, 187-197, doi: 10.1021/acscchembio.1c00844, 2022
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【受賞・表彰】

- 1) Osada, H., The People's Government of Jilin Province Changbai Mountain Friendship Award, 2021年12月10日
- 2) Minamoto, C., Miyazawa, K., Tabuchi, M., Hirano, M., Mizuno, M., Yoshizako, M., Torii, Y., Asano, Y., Sato, T., Kawatani, M., Osada, H., Maeda, H., Goto, S. 2021 Wayne G. Watson Award for Biologic or Experimental Research, 2021年6月25日
- 3) 長田裕之, 令和3年春の褒章, 紫綬褒章, 内閣府、2021年4月28日

【アウトリーチ活動】

- 1) 長田裕之, 第9回 DSANJ Digital Bio Conference 2022年1月26-28日 WEB開催
- 2) 長田裕之, 加藤記念バイオサイエンス振興財団, 若者へのメッセージ
(https://www.katokinen.or.jp/msg/msg_from_osada.html)
- 3) 理研一般公開開催時(埼玉, 2019年4月20日)に、一般の方々(約200名)に対して天然物化学研究の紹介や体験イベントを行った。
- 4) JST企画 科学の甲子園エクスカッション(理化学研究所、2019年3月18日)にて、参加高校生(約40名)に対して、研究施設の見学と、関連領域であるケミカルバイオロジーの説明を行った。
- 5) 東京都立小松川高校(理数系部活)の理化学研究所見学(2018年12月21日)において、引率教員を含めおよそ20人に対して、研究施設の見学と、関連領域であるケミカルバイオロジーの説明を行った。
- 6) 一般の方を対象にした理化学研究所による和光地区見学ツアー(2018年12月14日開催)において、14人の参加者に対して研究施設の見学と、関連領域であるケミカルバイオロジーの説明を行った。
- 7) 佐賀県立佐賀西高校1年生の理化学研究所見学(2018年8月3日)において、引率教員を含めおよそ15人に対して、研究施設の見学と、関連領域であるケミカルバイオロジーの説明を行った。