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Current Status: Assistant Professor
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Date of Birth: 13 May 1991
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Education:

04/2016-03/2019	Department of Computer Science, School of Computing, Tokyo Institute of Technology, D.Eng.
04/2014-03/2016	Department of Computer Science, Graduate School of Information Science and Engineering, Tokyo Institute of Technology, M.Eng.
04/2010-03/2014	Department of Computer Science, Faculty of Engineering, Tokyo Institute of Technology, B.Eng.

Employment:

10/2024-present	Assistant Professor, Institute of Science Tokyo
09/2020-present	Part-time Lecturer, Tokyo Tech Innovation
03/2020-09/2024	Assistant Professor, Tokyo Institute of Technology
11/2019-03/2020	Part-time Lecturer, Tokyo Institute of Technology
04/2019-03/2020	JSPS Research Fellow (PD), Japan Society for the Promotion of Science
04/2017-03/2019	JSPS Research Fellow (DC2), Japan Society for the Promotion of Science

Grants:

FY2023-FY2026	“Designing cyclic peptide with target protein selection based on mixed-solvent molecular dynamics simulation”, JSPS KAKENHI (grant-in-aid for Scientific Research (B)), 23H03495/23K28185, PI, 18 590 000 yen

FY2022-FY2024 "Development of chemical substructure-based virtual screening method for huge compound library", JSPS KAKENHI (grant-in-aid for Scientific Research (B)), 22H03684/23K24939, 17 030 000 yen
(PI: Yutaka Akiyama)

FY2020-FY2022 "Comprehensive prediction of cryptic binding sites by multi-task deep learning", JSPS KAKENHI (grant-in-aid for young researchers), 20K19917, PI, 4 290 000 yen

FY2020 "Computer-aided lead optimization with cosolvent molecular dynamics (CMD)", Grant for young researcher, School of Computing, Tokyo Institute of Technology, PI, 496 000 yen

FY2019 "Improvement of cosolvent MD which enables the systematic search of binding sites and the novel screening way of drug candidates", JSPS KAKENHI (grant-in-aid for JSPS fellows), 19J00878, PI, 1 820 000 yen

FY2017-FY2018 "Development of divide-and-conquer based docking method using common partial structures of hundreds of millions of compounds", JSPS KAKENHI (grant-in-aid for JSPS fellows), 17J06897, PI, 2 100 000 yen

Awards:

03/2021 2019 Education Award of Excellence,
Tokyo Institute of Technology (as a member out of 17 members)

02/2020 Seiichi Tejima Doctoral Dissertation Award,
Tokyo Institute of Technology.

12/2017 Grand Prize (Schrodinger K.K. Prize),
4th Computer-Aided Drug Discovery Contest.

07/2015 Student Encouragement Prize,
2nd Computer-Aided Drug Discovery Contest.

06/2015 2014 SIGBIO Best Student Presentation Award, IPSJ SIGBIO.

07/2014 Student Encouragement Prize,
1st Computer-Aided Drug Discovery Contest.

03/2014 2013 Tokyo Institute of Technology Academic Excellence Awards,
Tokyo Institute of Technology.

09/2009 Bronze Prize, 2009 High School Chemistry Grand Prix.

Current Research Interests:

Molecular Dynamics, Computational Biology, Bioinformatics, Structural Biology, Protein-Ligand Docking, Protein-Ligand Interaction, Computational Drug Discovery, Virtual Screening, Structure-based Virtual Screening, Machine Learning

Publications:

Peer-reviewed Journal Papers

1. Jianan Li, **Keisuke Yanagisawa**, Yutaka Akiyama. "CycPeptMP: enhancing membrane permeability prediction of cyclic peptides with multi-level molecular features and data augmentation", *Briefings in Bioinformatics*, 25: bbae417, 08/2024.
2. **Keisuke Yanagisawa**, Takuya Fujie, Kazuki Takabatake, Yutaka Akiyama. "QUBO Problem Formulation of Fragment-Based Protein-Ligand Flexible Docking", *Entropy*, 26: 397, 04/2024.
3. Genki Kudo†, **Keisuke Yanagisawa**†, Ryunosuke Yoshino, Takatsugu Hirokawa. "AAp-MSMD: Amino Acid Preference Mapping on Protein-Protein Interaction Surfaces Using Mixed-Solvent Molecular Dynamics", *Journal of Chemical Information and Modeling*, 63: 7768-7777, 12/2023. (†: Contributed equally)
4. Jianan Li, **Keisuke Yanagisawa**, Masatake Sugita, Takuya Fujie, Masahito Ohue, Yutaka Akiyama. "CycPeptMPDB: A Comprehensive Database of Membrane Permeability of Cyclic Peptides", *Journal of Chemical Information and Modeling*, 63: 2240-2250, 03/2023.
5. Masatake Sugita, Takuya Fujie, **Keisuke Yanagisawa**, Masahito Ohue, Yutaka Akiyama. "Lipid composition is critical for accurate membrane permeability prediction of cyclic peptides by molecular dynamics simulations", *Journal of Chemical Information and Modeling*, 62: 4549-4560, 09/2022.
6. **Keisuke Yanagisawa**, Rikuto Kubota, Yasushi Yoshikawa, Masahito Ohue, Yutaka Akiyama. "Effective protein-ligand docking strategy via fragment reuse and a proof-of-concept implementation", *ACS Omega*, 7: 30265-30274, 08/2022.
7. **Keisuke Yanagisawa**, Ryunosuke Yoshino, Genki Kudo, Takatsugu Hirokawa. "Inverse Mixed-Solvent Molecular Dynamics for Visualization of the Residue Interaction Profile of Molecular Probes", *International Journal of Molecular Sciences*, 23: 4749, 04/2022.
8. Kazuki Takabatake, **Keisuke Yanagisawa**, Yutaka Akiyama. "Solving Generalized Polyomino Puzzles Using the Ising Model", *Entropy*, 24: 354, 02/2022.
9. Jianan Li, **Keisuke Yanagisawa**, Yasushi Yoshikawa, Masahito Ohue, Yutaka Akiyama. "Plasma protein binding prediction focusing on residue-level features and circularity of cyclic peptides by deep learning", *Bioinformatics*, 38: 1110-1117, 02/2022.
10. **Keisuke Yanagisawa**. "Virtual Screening Methods with a Protein Tertiary Structure for Drug Discovery", *JSBi Bioinformatics Review*, 2: 76-86, 10/2021. (in Japanese)
11. Kazuki Takabatake, Kazuki Izawa, Motohiro Akikawa, **Keisuke Yanagisawa**, Masahito Ohue, Yutaka Akiyama. "Improved Large-Scale Homology Search by Two-step Seed Search Using Multiple Reduced Amino Acid Alphabets", *Genes*, 12, 1455, 09/2021.
12. Masatake Sugita, Satoshi Sugiyama, Takuya Fujie, Yasushi Yoshikawa, **Keisuke Yanagisawa**, Masahito Ohue, Yutaka Akiyama. "Large-Scale Membrane Permeability Prediction of Cyclic

Peptides Crossing a Lipid Bilayer Based on Enhanced Sampling Molecular Dynamics Simulations", *Journal of Chemical Information and Modeling*, 61, 3681–3695, 07/2021.

13. **Keisuke Yanagisawa**, Yoshitaka Moriwaki, Tohru Terada, Kentaro Shimizu. "EXPRORER: Rational cosolvent set construction method for cosolvent molecular dynamics using large-scale computation", *Journal of Chemical Information and Modeling*, 61, 2744–2753, 06/2021.
14. Masahiro Mochizuki, Shogo D. Suzuki, **Keisuke Yanagisawa**, Masahito Ohue, Yutaka Akiyama. "QEX: Target-specific druglikeness filter enhances ligand-based virtual screening", *Molecular Diversity*, 23, 11–18, 02/2019.
15. Takashi Tajimi, Naoki Wakui, **Keisuke Yanagisawa**, Yasushi Yoshikawa, Masahito Ohue, Yutaka Akiyama: "Computational prediction of plasma protein binding of cyclic peptides from small molecule experimental data using sparse modeling techniques", *BMC Bioinformatics*, 19, 527, 12/2018. (14 pages)
16. **Keisuke Yanagisawa**, Shunta Komine, Rikuto Kubota, Masahito Ohue, Yutaka Akiyama. "Optimization of memory use of fragment extension-based protein-ligand docking with an original fast minimum cost flow algorithm", *Computational Biology and Chemistry*, 74, 399–406, 06/2018.
17. Takanori Hayashi, Yuri Matsuzaki, **Keisuke Yanagisawa**, Masahito Ohue, Yutaka Akiyama. "MEGADOCK-Web: an integrated database of high-throughput structure-based protein-protein interaction predictions", *BMC Bioinformatics*, 19, 62, 05/2018. (12 pages)
18. **Keisuke Yanagisawa**, Shunta Komine, Shogo D. Suzuki, Masahito Ohue, Takashi Ishida, Yutaka Akiyama. "Spresso: An ultrafast compound pre-screening method based on compound decomposition", *Bioinformatics*, 33, 3836–3843, 03/2017.
19. Shuntaro Chiba, Takashi Ishida, Kazuyoshi Ikeda, Masahiro Mochizuki, Reiji Teramoto, Y-h. Taguchi, Mitsuo Iwadate, Hideaki Umeyama, Chandrasekaran Ramakrishnan, A. Mary Thangakani, D. Velmurugan, M. Michael Gromiha, Tatsuya Okuno, Koya Kato, Shintaro Minami, George Chikenji, Shogo D. Suzuki, **Keisuke Yanagisawa**, Woong-Hee Shin, Daisuke Kihara, Kazuki Z. Yamamoto, Yoshitaka Moriwaki, Nobuaki Yasuo, Ryunosuke Yoshino, Sergey Zozulya, Petro Borysko, Roman Stavniichuk, Teruki Honma, Takatsugu Hirokawa, Yutaka Akiyama, Masakazu Sekijima, "An iterative compound screening contest method for identifying target protein inhibitors using the tyrosine-protein kinase Yes", *Scientific Reports*, 7, 12038, 09/2017. (13 pages)
20. Shuntaro Chiba, Kazuyoshi Ikeda, Takashi Ishida, M. Michael Gromiha, Y-h. Taguchi, Mitsuo Iwadate, Hideaki Umeyama, Kun-Yi Hsin, Hiroaki Kitano, Kazuki Yamamoto, Nobuyoshi Sugaya, Koya Kato, Tatsuya Okuno, George Chikenji, Masahiro Mochizuki, Nobuaki Yasuo, Ryunosuke Yoshino, **Keisuke Yanagisawa**, Tomohiro Ban, Reiji Teramoto, Chandrasekaran Ramakrishnan, A. Mary Thangakani, D. Velmurugan, Philip Prathipati, Junichi Ito, Yuko Tsuchiya, Kenji

Mizuguchi, Teruki Honma, Takatsugu Hirokawa, Yutaka Akiyama, Masakazu Sekijima. “Identification of potential inhibitors based on compound proposal contest: Tyrosine-protein kinase Yes as a target”, *Scientific Reports*, 5, 17209, 12/2015. (13 pages)

21. **Keisuke Yanagisawa**, Takashi Ishida, Yutaka Akiyama. “Drug Clearance Pathway Prediction Based on Semi-supervised Learning”, *IPSJ Transactions on Bioinformatics*, 8, 21–27, 08/2015.

Peer-reviewed International Conference Papers

22. Kazuki Takabatake, Kazuki Izawa, Motohiro Akikawa, **Keisuke Yanagisawa**, Masahito Ohue, Yutaka Akiyama. “Improved Homology Search for Metagenomic Analysis by Two-Step Seed Search with Reduced Amino Acid Alphabets”, *The 10th International Conference on Bioinformatics and Biomedical Science (ICBBS2021)*, 10/2021.
23. Kazuya Isawa, **Keisuke Yanagisawa**, Masahito Ohue, Yutaka Akiyama. “Antisense oligonucleotide activity analysis based on opening and binding energies to targets”, In *Proceedings of the 27th International Conference on Parallel and Distributed Processing Techniques and Applications (PDPTA’21)*, 07/2021.
24. Masahito Ohue, Ryota Ii, **Keisuke Yanagisawa**, Yutaka Akiyama. “Molecular activity prediction using graph convolutional deep neural network considering distance on a molecular graph", In *Proceedings of the 25th International Conference on Parallel and Distributed Processing Techniques and Applications (PDPTA'19)*, 07/2019.
25. Takashi Tajimi, Naoki Wakui, **Keisuke Yanagisawa**, Yasushi Yoshikawa, Masahito Ohue, Yutaka Akiyama. “Computational prediction of plasma protein binding of cyclic peptides from small molecule experimental data using sparse modeling techniques”, *The 29th International Conference on Genome Informatics (GIW 2018)*, 12/2018.
26. **Keisuke Yanagisawa**, Shunta Komine, Rikuto Kubota, Masahito Ohue, Yutaka Akiyama. “Optimization of memory use of fragment extension-based protein-ligand docking with an original fast minimum cost flow algorithm”, *The 16th Asia Pacific Bioinformatics Conference (APBC2018)*, 01/2018.
27. Takanori Hayashi, Yuri Matsuzaki, **Keisuke Yanagisawa**, Masahito Ohue, Yutaka Akiyama. “MEGADOCK-Web: an integrated database of high-throughput structure-based protein-protein interaction predictions”, *The 16th Asia Pacific Bioinformatics Conference (APBC2018)*, 01/2018.
28. **Keisuke Yanagisawa**, Shunta Komine, Shogo D. Suzuki, Masahito Ohue, Takashi Ishida, Yutaka Akiyama. “ESPRESSO: An ultrafast compound pre-screening method based on compound decomposition”, *The 27th International Conference on Genome Informatics (GIW 2016)*, 10/2016.

International Conferences (without peer review)

29. **Keisuke Yanagisawa**, Ryunosuke Yoshino, Genki Kudo, Takatsugu Hirokawa. "Quantitative Evaluation of Protein-Compound Substructure Interaction with Inverse Mixed-Solvent Molecular Dynamics Simulation", *21st IUPAB and 62nd BSJ joint congress 2024*, 06/2024. (poster presentation)
30. **Keisuke Yanagisawa**, Yoshitaka Moriwaki, Tohru Terada, Kentaro Shimizu. "Systematic construction of the cosolvents sets for cosolvent MD (CMD) with the large-scale simulation", *AHeDD2019/IPAB2019 Joint Symposium*, 11/2019. (oral presentation)
31. Masahito Ohue, Takanori Hayashi, Yuri Matsuzaki, **Keisuke Yanagisawa**, Yutaka Akiyama. "Megadock-Web: An Integrated Database of High-Throughput Structure-Based Protein-Protein Interaction Predictions", *Biophysical Society 63rd Annual Meeting*, 2792-Pos, 03/2019. (poster presentation)
32. **Keisuke Yanagisawa**, Shunta Komine, Shogo D. Suzuki, Masahito Ohue, Takashi Ishida, Yutaka Akiyama. "Spresso: An ultrafast compound pre-screening method based on compound fragmentation", *Biophysical Society 62nd Annual Meeting*, 02/2018. (poster presentation)
33. Rikuto Kubota, **Keisuke Yanagisawa**, Masahito Ohue, Yutaka Akiyama. "Toward efficient protein-ligand docking for virtual screening by reuse of fragments", *The 16th Asia Pacific Bioinformatics Conference (APBC2018)*, Poster C5, 01/2018. (poster presentation)
34. **Keisuke Yanagisawa**, Shunta Komine, Masahito Ohue, Takashi Ishida, Yutaka Akiyama. "Fast pre-filtering for virtual screening based on compound fragmentation", *3rd IIT Madras–Tokyo Tech Joint Symposium on Algorithms and Applications of Bioinformatics*, P34, 11/2015. (poster presentation)