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Keisuke Yanagisawa

Research Fellow (PD), Japan Society for the Promotion of Science (JSPS)

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Current Status: Postdoctoral researcher
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Date of Birth: 13 May 1991
Place of Birth: Tokyo, Japan
Citizenship: Japan

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:

04/2019-present	JSPS Research Fellow (PD)
04/2017-03/2019	JSPS Research Fellow (DC2)

Grants:

FY2017-FY2018	JSPS KAKENHI (grant-in-aid for JSPS fellows), “Development of divide-and-conquer based docking method using common partial structures of hundreds of millions of compounds”, PI, $19 000

Awards:

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:

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

Publications:

Peer-reviewed Journal Papers

1. 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, 2019.
2. 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, 2018.
3. **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, 2018.
4. 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, 2018.
5. **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, 2017.

6. 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, 2017.
7. 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, 2015.
8. **Keisuke Yanagisawa**, Takashi Ishida, Yutaka Akiyama. "Drug Clearance Pathway Prediction Based on Semi-supervised Learning", *IPSJ Transactions on Bioinformatics*, 8, 21–27, 2015.

Peer-reviewed International Conference Papers

1. 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)*, 2018.
2. **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)*, 2018.
3. 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)*, 2018.
4. **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)*, 2016.