

Keisuke Yanagisawa

Department of Computer Science, School of Computing, Tokyo Institute of Technology

Education Academy of Computational Life Sciences (ACLS), Tokyo Institute of Technology

Current Status: PhD student

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Date of Birth: 13 May 1991

Place of Birth: Tokyo, Japan

Citizenship: Japan

Education:

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

Employment:

- 04/2017-present 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:

- 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:

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. **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*. (Epub ahead of print)
2. Shuntaro Chiba, Kazuyoshi Ikeda, Takashi Ishida, M. Michael Gromiha, Y-h. Taguchi, Mitsuo Iwadata, 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.
3. **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. **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)*, 7 pages, 2016.

Conference Papers

1. **Keisuke Yanagisawa**, Masahito Ohue, Takashi Ishida, Yutaka Akiyama. “Compound filtering by estimation of the candidate compound’s upper limit size using target protein structure”, *IPSJ SIG Technical Report*, 2016-BIO-49(6), 1–7, 2017.
2. **Keisuke Yanagisawa**, Shunta Komine, Shogo D. Suzuki, Masahito Ohue, Takashi Ishida, Yutaka Akiyama. “ESPRESSO: An ultrafast compound pre-screening method based on compound decomposition”, *IPSJ SIG Technical Report*, 2016-BIO-46(18), 1–7, 2016.
3. Shogo D. Suzuki, **Keisuke Yanagisawa**, Masahito Ohue, Takashi Ishida, Yutaka Akiyama. “Prediction of Human c-Yes Kinase Inhibitors by SVM and Deep Learning”, *IPSJ SIG Technical Report*, 2015-BIO-42(36), 1–7, 2015.
4. **Keisuke Yanagisawa**, Takashi Ishida, Yuichi Sugiyama, Yutaka Akiyama. “Drug clearance pathway prediction based on semi-supervised learning”, *IPSJ SIG Technical Report*, 2014-BIO-41(11), 1–6, 2015.
5. **Keisuke Yanagisawa**, Takashi Ishida, Yutaka Akiyama. “Drug clearance pathway prediction using semi-supervised learning”, *IPSJ SIG Technical Report*, 2014-BIO-38(10), 1–6, 2014.

Poster Presentations

1. **Keisuke Yanagisawa**, Shogo D. Suzuki, Shunta Komine, Masahito Ohue, Takashi Ishida, Yutaka Akiyama. “ESPRESSO: An ultrafast compound pre-screening method with segmented compounds”, *CBI Annual Meeting 2016*, P2-19, 2016.
2. **Keisuke Yanagisawa**, Shogo D. Suzuki, Shunta Komine, Masahito Ohue, Takashi Ishida, Yutaka Akiyama. “ESPRESSO: An ultrafast compound pre-screening method based on compound segmentation”, *Informatics in Biology, Medicine and Pharmacology 2016*, P65, 2016.
3. **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, 2015.
4. **Keisuke Yanagisawa**, Shunta Komine, Masahito Ohue, Takashi Ishida, Yutaka Akiyama. “Fast pre-filtering for virtual screening based on ligand decomposition”, *21st Young Researchers Forum for Pharmaceutical Technology Innovation*, P-6, 2015.
5. **Keisuke Yanagisawa**, Shunta Komine, Masahito Ohue, Takashi Ishida, Yutaka Akiyama. “Fast pre-filtering for virtual screening based on compound decomposition”, *Informatics in Biology, Medicine and Pharmacology 2015*, P58, 2015.