Kenichiro Takaba

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Research Interests

Drug design, Molecular dynamics simulation, Fragment molecular orbital method, Free energy calculations, De novo drug design, Protein engineering, Machine learning potentials (neural network potentials), Machine learning (graph neural networks, reinforcement learning, active learning, transfer learning, etc.), Large language models

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Education

- **2016-2020**: Ph.D. in Physics, The University of Tokyo, Japan
  Edge expansion parallel cascade selection molecular dynamics simulation (eePaCS-MD) for investigating protein dynamics
- **2010-2012**: M.S. in Physics, The University of Tokyo, Japan
  Theoretical study of the protonation states of H+-PPase using molecular dynamics simulations
- **2006-2010**: B.S. in Engineering Science, University of Tsukuba, Japan

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Work Experience

- **2012.04-Present**: Principal Scientist, Asahi Kasei Pharma Corporation
  - Structure-based and ligand-based drug discovery projects for small molecules, peptides and antibodies
  - Infrastructure development for computational tools (e.g. automated docking, QSAR/QSPR, de-novo design)
  - Web service development
- **2022.04-2024.04**: Visiting Scientist, Memorial Sloan Kettering Cancer Center (Supervisor: John D. Chodera)
  - Development of open-source software for computer-aided drug discovery

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Technical Experience

- Expertise with biomolecular simulations, cheminformatics, and machine learning for drug discovery
- Expertise in using computational tools such as Maestro and MOE
- Expertise with Python and Unix shell scripts
- Expertise with open-source software packages such as RDKit, OpenMM, and machine learning frameworks (e.g. Scikit-learn, Pytorch)
- Fluent with GitHub for code sharing and development
- Experience with flask and SQLAlchemy to develop web services
- Experience with AWS for High Performance Computing (e.g. ParallelCluster)

Publications

- **On the design space between molecular mechanics and machine learning force fields**
  Appl. Phys. Rev. 2025, 12, 021304
  Wang Y, **Takaba K**, Chen MS, Wieder M, Xu Y, Zhu T, Zhang JZH, Nagle AM, Yu K, Wang X, Cole DJ, Rackers JA, Cho K, Greener JG, Eastman P, Martiniani S, Tuckerman ME
- **Machine-learned molecular mechanics force fields from large-scale quantum chemical data**
  Chem. Sci. 2024, 15, 12861-12878
  Takaba K, Friedman AJ, Cavender CE, Behara PK, Pulido I, Henry PK, MacDermott-Opeskin H, Iacovella CR, Nagle AM, Payne AM, Shirts MR, Mobley DL, Chodera JD, Wang Y
- **DrugGym: A testbed for the economics of autonomous drug discovery**
  bioRxiv 2024, bioRxiv:2024.05.28.596296
  Retchin M, Wang Y, **Takaba K**, Chodera JD

- **EspalomaCharge: Machine Learning-Enabled Ultrafast Partial Charge Assignment**
  J. Phys. Chem. A 2024, 128, 4160-4167
  Wang Y, Pulido I, **Takaba K**, Kaminow B, Scheen J, Wang L, Chodera JD
- **End-to-end differentiable construction of molecular mechanics force fields**
  Chem. Sci. 2022, 13, 12016-12033
  Wang Y, Fass J, Kaminow B, Herr JE, Rufa D, Zhang I, Pulido I, Henry MM, Bruce Macdonald HE , **Takaba K**, Chodera JD
- **Protein-ligand binding affinity prediction of cyclic-dependent kinase-2 inhibitors by dynamically averaged fragment molecular orbital-based interaction energy**
  J. Comput. Chem. 2022, 43, 1362-1371
  Takaba K, Watanabe C, Tokuhisa A, Akinaga Y, Ma B, Kanada R, Araki M, Okuno Y, Kawashima Y, Moriwaki H, Kawashita N, Honma T, Fukuzawa K, Tanaka S
- **FMODB: The World's First Database of Quantum Mechanical Calculations for Biomacromolecules Based on the Fragment Molecular Orbital Method**
  J. Chem. Inf. Model 2021, 61, 777-794
  Takaya D, Watanabe C, Nagase S, Kamisaka K, Okiyama Y, Moriwaki H, Yuki H, Sato T, Kurita N, Yagi Y, Takagi T, Kawashita N, **Takaba K**, Ozawa T, Takimoto-Kamimura M, Tanaka S, Fukuzawa K, Honma T
- **Discovery of 4,6- and 5,7-Disubstituted Isoquinoline Derivatives as a Novel Class of Protein Kinase C ζ Inhibitors with Fragment-Merging Strategy**
  J. Med. Chem. 2020, 63, 7143-7162
  Atobe M, Serizawa T, Yamakawa N, **Takaba K**, Nagano Y, Yamaura T, Tanaka E, Tazumi A, Bito S, Ishiguro M, Kawanishi M
- **Edge expansion parallel cascade selection molecular dynamics simulation for investigating large-amplitude collective motions of proteins**
  J. Chem. Phys. 2020, 152, 225101
  Takaba K, Tran DP, Kitao A

Invited Talks

- **Dec. 2025 (Honolulu, USA)**
  Pacifichem: *Machine-learned molecular mechanics force fields from large-scale quantum chemical data*
- **Nov. 2025 (Webinar, Japan)**
  468th CBI Seminar: *Machine-Learned Molecular Mechanics Force Fields Leveraging the OpenFF Ecosystem and Open Science*
- **May 2024 (Leiden, The Netherlands)**
  Alchemical Free Energy Workshop 2024: *Machine learned molecular mechanics force fields from large scale quantum chemical data*
- **Mar. 2020 (Kumamoto, Japan)**
  The 8th French-Japanese Workshop on Computational Methods in Chemistry: *Integrating MO, MD and Machine Learning to Accelerate Drug Discovery* (Suspended due to COVID-19)
- **Mar. 2018 (Tokyo, Japan)**
  392th CBI Seminar: *Application of Molecular Dynamics and Fragment Molecular Orbital Method in Drug Discovery*
- **2017 (Tokyo, Japan)**
  MOE Forum: *Validation of Supervised Molecular Dynamics and its Usefulness in Drug Discovery*

Books

- **Recent Advances of the Fragment Molecular Orbital Method** (2021, Springer)
  - Chapter: FMO Drug Design Consortium (pp. 127-181)
    Fukuzawa K, Tanaka S, Yagi Y, Kurita N, Kawashita N, **Takaba K**, Honma T

    - Chapter: Application of FMO for Protein-ligand Binding Affinity Prediction (pp. 281-294)
      Takaba K

Awards

- **MedChem Symposium** (2018), Poster Award
  構造ジェネレータを活用した化合物デザイン
  山口貴也、芹沢貴之、鷹羽健一郎、大川和史

Contributions

- 化学工学 (2023)
  創薬研究へのAI／機械学習の活用
  山口貴也, 鷹羽健一郎, 大川和史
- アンサンブル (2021)
  エッジ拡張型並列カスケード選択分子動力学法（eePaCS-MD）を用いたタンパク質の動的構造探索
  鷹羽健一郎
- **MEDCHEM NEW** (2019)
  構造ジェネレータを活用した化合物デザイン
  山口貴也、芹沢貴之、鷹羽健一郎、大川和史

Other Activities

- **2017-2020**: Industry-Academia Collaboration Consortium
    - KBDD (K supercomputer-Based Drug Discovery project by Biogrid parama consortium)
    - FMODD (FMO Drug Design Consortium)
      KBDD Working Group Leader: *Method development integrating MD simulation and quantum chemical calculations in collaboration with KBDD*