Tokyo Tech Research Units

Advanced Computational Drug Discovery Unit

Overview

Molecular simulation is a method of calculating molecular activity to analyze the physical and chemical properties of compounds used in innovative drug discovery. Bioinformatics and systems biology are applied to analyze biological data using information-science methodologies such as artificial intelligence, bigdata analysis and machine learning. Integrating these methods, the Advanced Computational Drug Discovery Unit (ACDD) develops *in silico* technology for innovative drug discovery from an academic point of view through large-scale GPU computation using the TSUBAME supercomputer. Utilizing and complementing biochemical research conducted by pharmaceutical companies, the unit aims to establish methods of innovative drug discovery through open innovation with industries.

Research goals

It is essential for future innovative drug discovery to develop ideas and methods that facilitate beneficial collaboration between universities and corporations. ACDD sets the goal of realizing open innovation and aims to realize the establishment of an open drug discovery environment within five years. The unit will establish an advanced computational drug discovery model while focusing on the following three themes:

- Open utilization of the drug discovery environment by Tokyo Tech and pharmaceutical companies
- Establishment of an open-participation type *in silico* drug discovery contest
- Provision of education for industry professionals through the *in silico* drug discovery training program

Research Unit Leader **Masakazu Sekijima**

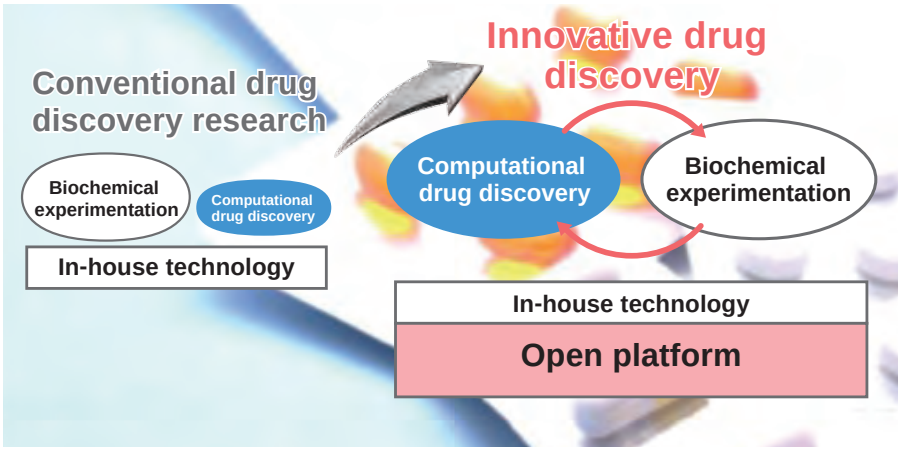
Profile

2016 Associate Professor, Institute of Innovative Research, Tokyo Institute of Technology
2009 Associate Professor, Global Scientific Information and Computing Center, Tokyo Institute of Technology
2008 Planning Officer, Planning Headquarters, National Institute of Advanced Industrial Science and Technology
2003 Research Scientist, Computational Biology Research Center, National Institute of Advanced Industrial Science and Technology
2002 Research Staff, Computational Biology Research Center, National Institute of Advanced Industrial Science and Technology
2002 Ph.D., Department of Biotechnology, Graduate School of Agricultural and Life Sciences, University of Tokyo

Unit members

- Professor Yutaka Akiyama
- Professor Akihiko Konagaya
- Associate Professor Takashi Ishida
- Associate Professor Shintaro Sengoku
- Visiting Associate Professor Teruki Honma
- Assistant Professor Masahito Ohue

Advanced Computational Drug Discovery Unit



A new Tokyo Tech research unit aiming to form an open platform for experimental studies on innovative drug discovery through integration of computational technology and experimental biochemistry

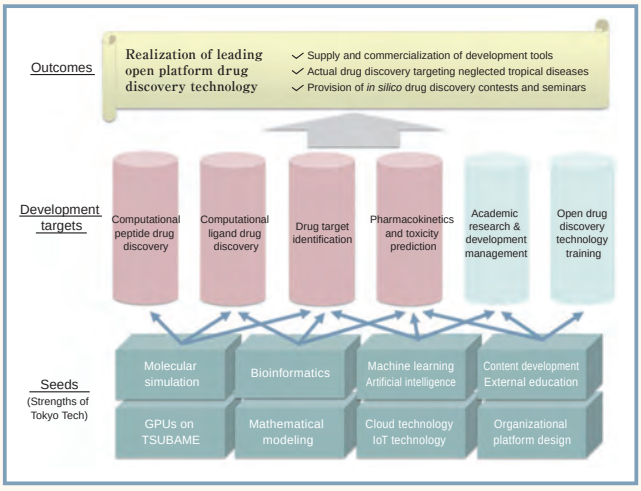
In line with the current trend, the concept of openness in drug discovery can be extended to other fields

Q Why was this research unit established?

Drug discovery is expensive, with development costs for a single drug often reaching USD 2.5 billion. In addition, security is extremely important because any leak of information can cause significant damage to a project. This creates obstacles to effective collaboration between pharmaceutical companies and researchers. In addition, projects tend to be discontinued if good results are not achieved in a short period of time. This means that, due to insufficient trials and errors, companies and researchers cannot compile enough data to mutually complement each other's efforts. There are not enough people to analyze the data, which forces a dependence on methods that are not suitable for project conditions, thereby preventing breakthroughs. The Advanced Computational Drug Discovery Unit was established to take the initiative in making drug discovery technology open and accessible for universities and startups.

Q What are the strengths of this research unit?

We have shared our know-how with pharmaceutical companies. This came about through a consortium on neglected tropical diseases (NTDs), diseases for which therapeutic drug development has been slow because they affect mainly impoverished areas. The consortium focuses on drug discovery as a social contribution project. It is important to have serious discussion and two-way exchange of know-how on new drug discovery through collaboration between companies and universities. This concept of openness should not be limited to the field of drug discovery, but should be allowed to pervade other fields and industries.



Tokyo Tech uses the supercomputer TSUBAME to great advantage by employing it to identify compounds for drug discovery. Unit members are confident that the accumulation of experimental results in cooperation with partners who conduct biochemical research using the extracted compounds will prove highly effective for drug discovery.

Q What is the path to achieving the unit's goals?

After we establish the corporate consortium in April 2016, the unit will hold drug discovery contests for five years. These contests will be open to everyone. ACDD also plans to initiate *in silico* drug discovery training programs for working adults, and symposiums in cooperation with overseas universities such as the Indian Institute of Technology Madras. We believe that these projects will prove effective in developing highly skilled professionals and in establishing an open and accessible drug discovery environment that contributes to collaboration between universities and companies.

Meanwhile, the unit is transferring technical methods for drug discovery to the TSUBAME supercomputer, establishing servers for open and accessible drug discovery, sharing and comparing results, and applying data to advanced drug discovery utilizing a platform that will lead to the establishment of a stable foundation for research and development.

Contact us

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Advanced Computational Drug Discovery Unit

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