

Research commenced with Keio University to discover drugs using "Chemicals Informatics"

- Accelerating the development of small molecule drugs using materials informatics technology-

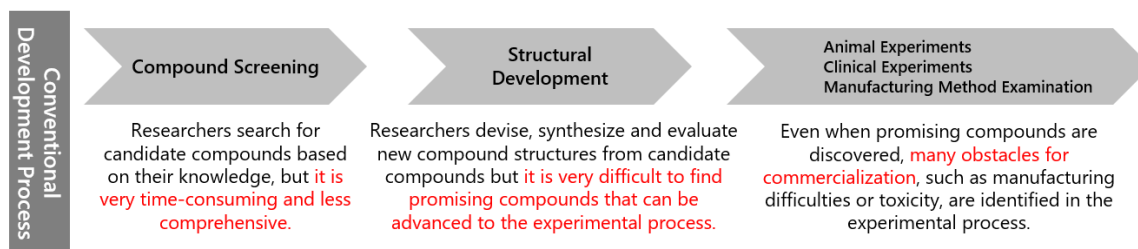
Tokyo, January 11, 2023 – Hitachi High-Tech Solutions Corporation ("Hitachi High-Tech Solutions"), in collaboration with Keio University Faculty of Pharmacy, Department of Pharmaceutical Sciences is commencing joint research that uses Materials Informatics (MI) (hereinafter, "the Research") to improve the efficiency of the development of small molecule drugs*1.

Hitachi High-Tech Solutions will be using the "Chemicals Informatics (CI)" MI tool not only by developing materials in the traditional chemical materials field but also in the field of drug discovery, to improve quality of care and QoL (Quality of Life) for people.

*1 Small molecule drug: A type of drug that has very small (low weight) molecules that are able to easily enter cells.

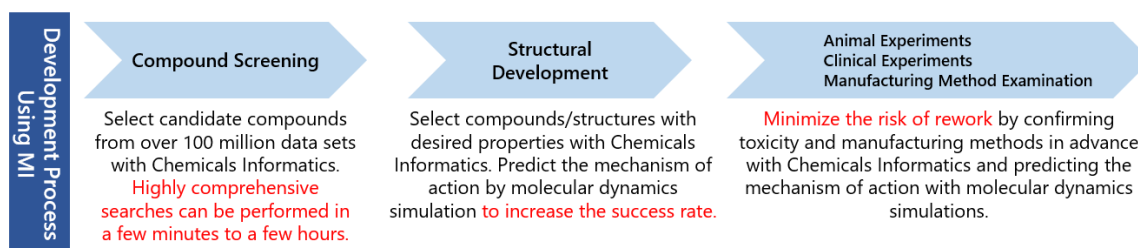
● Challenges in Conventional Small Molecule Drug Development

While it takes more than 10 years and huge costs for R&D process, the success rate is very low.



● Expected Benefits of Using MI(Materials Informatics) for Small Molecule Drug Development

Promoting new drug development and early commercialization by increasing R&D process efficiency, shortening timeframes and improving success rates.



■ Background to the Research

Small molecule drugs are mainstream drugs in the modern world, and in recent years, expectations for their use have increased, with the development of drugs such as molecular-targeted drugs that inhibit the action of proteins, which cause cancer². Traditionally, the process used to develop small molecule drugs has involved researchers using their knowledge and experience to select several potential compounds from an extensive library of existing compounds and then repeating experiments to adjust the structure of a compound and clarify the mechanism by which it will work, before moving on to clinical trial. As a result, more than a decade's worth of R&D has been conducted at a huge cost, with a very low success rate. MI is expected to solve these challenges by using information science techniques, such as AI, to improve the efficiency of compound and material development.

■ Overview of the Research

In the Research, Keio University Faculty of Pharmacy, Department of Pharmaceutical Sciences will use Hitachi High-Tech Solutions' CI to study the development of new drugs to act as selective inhibitors that will block enzymes that produce active sulfur molecules. We know that the production of a large quantity of active sulfur molecules in cells shows antioxidant effects, protein activity control and the generation of energy, etc. The development of small molecule drugs that inhibit the function of these enzymes is expected to lead to the elucidation of biological phenomena and the treatment of diseases such as cancer. The Research will use AI to conduct fast, comprehensive searches for promising compounds and potential structures based on the vast amount of data on compounds recorded in the CI, and then predict how the effects and mechanism will work using molecular dynamic simulations. This will help to improve the development of small molecule drugs in terms of a more efficient process, faster time scales and higher success rates, and will contribute to the development and early commercialization of new drugs.

Through this Research, Hitachi High-Tech Group will provide a practical demonstration of how CI, which to date has helped develop various materials in the chemical materials industry, can be applied to the development of pharmaceuticals and contribute to new drug development initiatives. In so doing, we will provide optimal solutions for creating social value and contribute to improving people's QoL (Quality of Life).

*2 Molecular-targeted drugs: A therapeutic agent designed to act only on specific molecules that cause disease.

Related Links

<https://www.hitachi-hightech.com/global/en/products/ict-solution/randd/ci/>

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About Hitachi High-Tech

Hitachi High-Tech, headquartered in Tokyo, Japan, is engaged in activities in a broad range of fields, including manufacture and sales of clinical analyzers, biotechnology products, and analytical instruments, semiconductor manufacturing equipment and analysis equipment. and providing high value-added solutions in fields of social & industrial infrastructures and mobility, etc. The company's consolidated revenues for FY 2021 were approx. JPY 576.8 billion [USD 5.1 billion]. For further information, visit <http://www.hitachi-hightech.com/global/>

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