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Introducing “Chemicals Informatics”: Software to Streamline New Product Research in the Chemical Industry

Tokyo, November 10, 2020 – Hitachi High-Tech Corporation today announced that Hitachi High-Tech Solutions Corporation (President: Masahiro Taniguchi / Hitachi High-Tech Solutions) is launching Chemicals Informatics – a new piece of software designed to help bring new high-value-added materials to market faster, as research and development (R&D) processes in the chemical sector has become more advanced and efficient.

In today's chemical industry, the development of new materials is intensifying in line with the acceleration of globalization. Companies centered around chemical manufacture are expected to bring products differentiated by new, high-value-added materials to the market quickly, and claim a high share of the target market in the process. However, it is not uncommon for the development of new materials to span decades and cost billions, or tens of billions, of yen. In response to these challenges, recent years have seen a focus on "materials informatics," which applies information science and technology such as data mining—analyzing large amounts of data to find useful information such as rules and regularities—and artificial intelligence (AI) to aid researchers and significantly increase the efficiency of R&D.
Hitachi High-Tech Solutions has developed Chemicals Informatics to help shorten the timescale and reduce the costs of developing new materials that have previously been researched and investigated over a significant amount of time by experienced and skilled researchers, thereby streamlining the R&D process.
Chemicals Informatics has the following key features:

1. A combination search method that helps researchers make new discoveries

By investigating potential compounds with our proprietary AI program that mimics the mechanism of biological evolution through DNA recombination and mutation, users can explore and efficiently discover new materials, chemicals, substitutes and more, in areas not covered by existing products.

2. A vast database of compounds to inspire new ideas

The combination search lets users mix and match different compounds from a wide pool of data spanning various fields, increasing the likelihood of finding new and

potential compounds that fit the intended purpose.
A database of more than a hundred million compounds, papers, patents and more, accumulated using proprietary NLP (Natural Language Processing)[*1] technology, along with compounds created by our proprietary AI technology, will help researchers to research and develop.

3. High security and stability that supports efficient research and development

The AI analysis infrastructure used for exploring new compounds is built on the highly secure and stable private cloud “ayamo” and is equipped with the GPU[*2] computing platform from US company NVIDIA enabling it to quickly and securely compute vast amounts of data, improving the productivity of R&D. An SSL-VPN[*3] gives users secure and easy access.

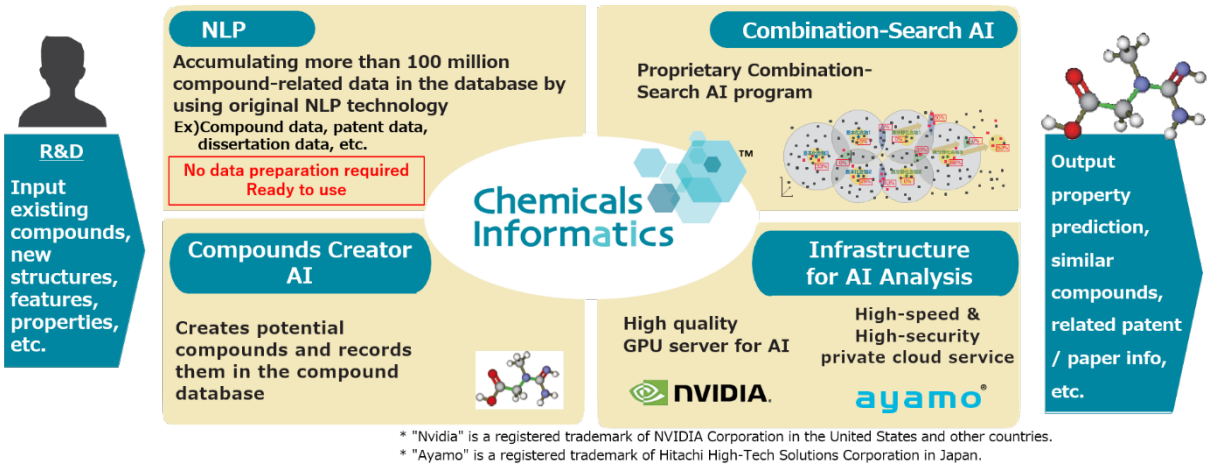
Hitachi High-Tech Solutions has long been providing solutions based on in-depth manufacturing knowledge and global business research capability to help refine customer business processes. With rapid advances to AI technology over recent years, we will continue to offer high-value-added services to help our customers be fast-moving and successful, through an enhanced lineup of business-ready products. Hitachi High-Tech Solutions will also work with Hitachi, Ltd.'s Materials Development Solution[*4] to promote digital innovations such as data-based solutions in a wide range of processes in the chemical industry, from R&D to manufacturing, enabling customers to harvest value from their data.
Going forward, Hitachi High-Tech Group is committed to providing solutions that contribute to resolving the issues facing our customers in the manufacturing sector, such as automating and improving productivity through the use of AI and IoT.

*1 Natural Language Processing (NLP): Analysis technology that correctly interprets meaning and punctuation in human languages, in the same way as a human being. It is used on computers and smartphones to convert Japanese characters between alphabets, among other uses.

*2 Graphics Processing Unit (GPU): A processor that computes the vast amounts of data required to render graphics. Due to its massive computing power, GPUs are being used generally for tasks that require prodigious amounts of computing, such as deep learning and scientific simulations. More recently, GPU deep learning ignited modern AI — the next era of computing — with the GPU acting as the brain of computers, robots and self-driving cars that can perceive and understand the world.

*3 Secure Sockets Layer Virtual Private Network (SSL-VPN): encryption technology that creates a virtual private network (VPN) for secure communications over the Internet (in web browser only).

*4 Materials Development Solution: One of Hitachi’s Lumada solutions accelerating digital transformation. A service that uses AI and other digital technologies to guide material development by analyzing a wide variety of material data through material informatics, thereby enhancing the materials development process.



[Chemicals Informatics overview image]

Comment from Masahiro Taniguchi, President of Hitachi High-Tech Solutions

We are delighted to be able to offer our long-standing expertise in manufacturing and AI technology to research developers through Chemicals Informatics. Chemicals Informatics is an innovative product that will not only accelerate the R&D process for various chemical substances, but also has the potential to help uncover undiscovered and potential compounds. Chemicals Informatics combines our own unique cloud technology with an NVIDIA product already adopted by AI research institutions around the world for AI analysis computing, enabling safe, fast and stable processing. We hope to contribute to society by helping our customers create new value through this product.

Comment from Masataka Osaki, Vice President of Corporate Sales and NVIDIA Japan Country Manager

NVIDIA is excited for the release of Chemicals Informatics, which is supported by NVIDIA's DGX system, an essential tool for AI research. The innovative NVIDIA V100 Tensor core GPUs featured in DGX will deliver dramatically faster training times for deep learning. We hope our state-of-the-art AI system will contribute to Chemicals Informatics for streamlining the chemistry research process.

Chemicals Informatics website

https://www.hitachi-hightech.com/hsl/products/ict/cloud/ci

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