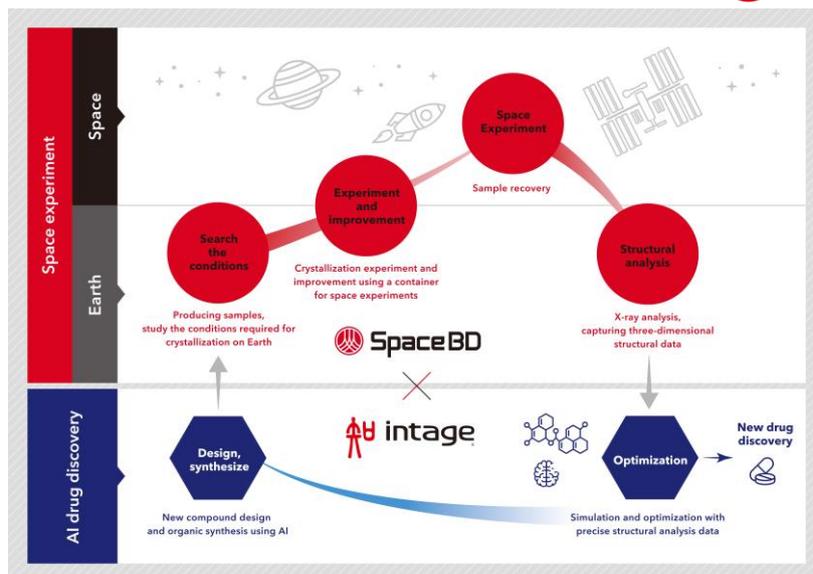


Intage Healthcare and Space BD
World's first* collaboration
between AI drug discovery
and commercial space experiment
Joint study commences towards providing
support and service in drug discovery research
Launch of sample scheduled by the end of 2022

*Source: Space BD



Intage Healthcare and Space BD will commence a joint research project linking their services: “Deep Quartet”, an AI platform for developing new drugs, and “high-quality protein crystal analysis”, a service that leverages the unique microgravity environment in outer space. A launch of the sample in 2022 and experiments in space will be carried out. After the sample is recovered, an X-ray crystal analysis and an AI calculated optimization will be performed. The goal for the future is to provide the world’s first service that supports drug discovery research using precise structural data gained from experiments conducted in space and AI-designed compounds.



[Image of the collaboration between “Deep Quartet”, an AI drug discovery platform, and the “space experiment and high-quality protein crystal growth service”]

The objective of this joint research project is to develop the technology for optimizing compounds in drug discovery research. Experiments conducted in space and AI drug discovery technology will unravel the interaction between new pharmaceutical compounds designed with AI drug discovery technology and disease-related proteins.

Using the unique microgravity environment at the Japanese experiment module ISS “Kibo”, high-quality protein crystals can be generated and precise structural data that cannot be captured through experiments on Earth can be obtained. The extremely precise structural data and AI drug discovery technology will be applied to the development of optimization technology for compounds, including ‘weak intermolecular force’^(*) which is considered vital to drug design. Results of the joint research will support development costs and contribute to streamlining the development period in drug discovery research.

Intage Healthcare and Space BD will work together on this joint research project and will continue to offer their respective services to pharmaceutical companies and venture firms involved in drug discovery.

(*) In pharmaceutical molecular design, it is essential for molecules (compounds) to have a strong bond to the target protein. In recent optimization studies of lead compounds, certain weak intermolecular force, such as CH-n interaction, are considered to play a vital role.

【About “Deep Quartet”】

The AI drug discovery platform “Deep Quartet” is a service jointly provided by Intage Healthcare Inc., the Institute for Theoretical Medicine, Inc., and Affinity Science Corporation. Deep Quartet is a series of flows combining deep reinforcement learning⁽¹⁾, LigandScout⁽²⁾,

which is a software that creates pharmacophore models, and CzeekS⁽³⁾, a technology based on machine learning that allows comprehensive target estimation. Adding the knowledge of medicinal chemists⁽⁴⁾ at pharmaceutical companies, the four elements form a quartet for the AI drug discovery platform. The compound that is designed can be synthesized through the one-stop service offered a partner company, KNC Laboratories Co., Ltd. Details about the technology or an introduction to case studies are offered in the following theses:

- Design and synthesis of DDR1 inhibitors with a desired pharmacophore using deep generative models. ChemMedChem 2021; 16:955–58.
- Strategies for design of molecular structures with a desired pharmacophore using deep reinforcement learning. Chem Pharm Bull (Tokyo) 2020; 68(3):227-33.

【High-quality protein crystal experiment on ISS “Kibo”】

Space BD is the sole private partner involved in the high-quality protein crystal growth business conducted over ten years by JAXA on “Kibo”. Space BD offers domestic and international firms and research institutes the opportunity to conduct experiments in space. Through the collaboration with Maruwa Foods and Biosciences, Inc., a company that has been supporting JAXA’s space experiments from the initial stage, Space BD can also examine the conditions for crystallization, provide space transport, recover the crystals, offer structural analysis, as well as propose molecular design.



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Comment from Dire Director Ryuta Murakami,
Data Science Division, Drug Discovery Support Unit Intage Healthcare Inc.



We have been working with our partners to provide research support in drug discovery using AI with the focus on the practical elements. The collaboration with Space BD links space experiments with AI drug discovery, which has entered the pragmatic application phase. We are confident that this partnership will accelerate drug discovery domestically as well as abroad.

Comment from Shokiki Kawata, Business Development Life-science R&D project Space BD



It is truly exciting to provide an innovative service that takes on the challenge of streamlining drug discovery research by leveraging space and digital technology. I hope to continue finding links with technological seeds that have never been considered for use in space and to identifying new needs in the market so we can expand opportunities in the space business.

【For reference】

A sample transported to the ISS for the experiment to generate low-temperature high-quality protein crystal



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Amylase protein crystal generated at the ISS (left) and on Earth (right)



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【Intage Healthcare Inc.】 <https://www.intage-healthcare.co.jp/>

The core business of Intage Healthcare Inc. is to provide marketing research, pharmaceutical development, post-production and sales survey, and operational safety support in healthcare. Solutions are delivered with the integrated efforts of the firms* that support the Intage Group's mission. Any healthcare challenge is dealt with by supporting optimal decisions based on the value of medical consumer data.

* Kyowa Kikaku Ltd., Intage Real World Inc., Plamed Inc., and Plamed Korea Co., Ltd.

【Space BD Inc.】 <https://space-bd.com>

Space BD is a leading Japanese company focusing on business development to drive the commercialization of space. Since its foundation in 2017, Space BD plays a unique and important role as business development professionals in the industry and provides optimal solutions and a one-stop service to every customer. With a performance record of over 50 satellite projects and over 100 orders to date, Space BD continues to expand its support for customers exploring possibilities in space.

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