Next-generation Chemical Reaction Analysis Using Quantum-integrated Chemistry Platform “QIDO” in Collaboration with Chugai Pharmaceutical

Mitsui & Co., Ltd. (“Mitsui”, Head Office: Tokyo, President and CEO: Kenichi Hori), together with the U.S. computational chemistry software company Quantum Simulation Technologies, Inc. (“QSimulate”, CEO: Toru Shiozaki), has decided, through an initiative with Chugai Pharmaceutical Co., Ltd. (“Chugai”, Head Office: Tokyo, Representative Director, President and CEO: Osamu Okuda), to expand the functionality of QIDO*1, a quantum-integrated chemistry platform, to analyze complex molecules and chemical reactions for pharmaceutical research. Mitsui will be responsible for defining specific research themes, advancing the overall project, and leading business development based on Chugai’s research priorities and evaluations of QIDO utilization. The goal is to make functions developed through this initiative available to a wide range of pharmaceutical and chemical companies as QIDO product features. As outlined below, a related research theme based on the use of QIDO has also been selected for the JHPC-quantum test user program.

JHPC-quantum is the commonly used name for the NEDO-commissioned project “Research and Development of Quantum-Supercomputers Hybrid Platform for Exploration of Uncharted Computable Capabilities” (Representative Project Leader: Mitsuhisa Sato), which is being carried out under NEDO’s “Research and Development Project of the Enhanced Infrastructures for Post-5G Information and Communication Systems” (JPNP20017), supported by the Ministry of Economy, Trade and Industry (METI). JHPC-quantum is a pioneering project that aims to expand the computable domain through the integration of quantum computers and high-performance computing. As part of this project, a Test User Program is being conducted to explore specific use cases. A research theme based on the use of QIDO was recently selected for this program, with Chugai as the lead proposer, QSimulate as a co-proposer, and Mitsui as a collaborating partner. This selection signifies that the initiative using QIDO was evaluated, following a review under a national research and development project, as a proposal with concrete value, utility, and technical feasibility.

One of the challenges to emerge from the growing complexity of pharmaceutical research in recent years is achieving high accuracy when predicting chemical reactions computationally. Greater predictive accuracy can improve research efficiency by reducing the number of costly and time-consuming experiments

needed.

A key step toward addressing this challenge will be accurate computation and prediction of the energy states of electrons involved in reactions. This initiative will verify the potential of quantum computing, which is expected to be highly effective in performing such computations. In addition to using supercomputers and GPUs for large-scale reaction analyses, the initiative will also explore the use of Quantinuum's quantum computer Reimei*2, which was recently upgraded to handle more complex computations. Using QIDO to integrate and automate these calculations makes this one of the most advanced initiatives in the world.

In addition to pharmaceutical development, the analysis of complex chemical reactions is also a priority for R&D in such areas as catalysts, electronic and functional materials, resins, and additives. Mitsui has highlighted "Industrial Business Solution 2.0" in its Medium-term Management Plan 2029. By providing QIDO functions across a wide range of fields, Mitsui will contribute to solving industrial challenges in various fields through digital technologies, and ultimately to solving broader social issues.

*1: QIDO stands for "Quantum-Integrated Discovery Orchestrator." It is a computational chemistry platform created to support R&D focused on new drugs and materials. It combines high-precision analysis of chemical reactions using conventional computers with the capabilities needed when using quantum computers.
*2: Reimei: A Quantinuum quantum computer installed at RIKEN. It has been upgraded to System Model H2, thereby raising the number of qubits used in computations from 20 to 56. This and other improvements will allow the computer to handle complex calculations using larger amounts of information than before.