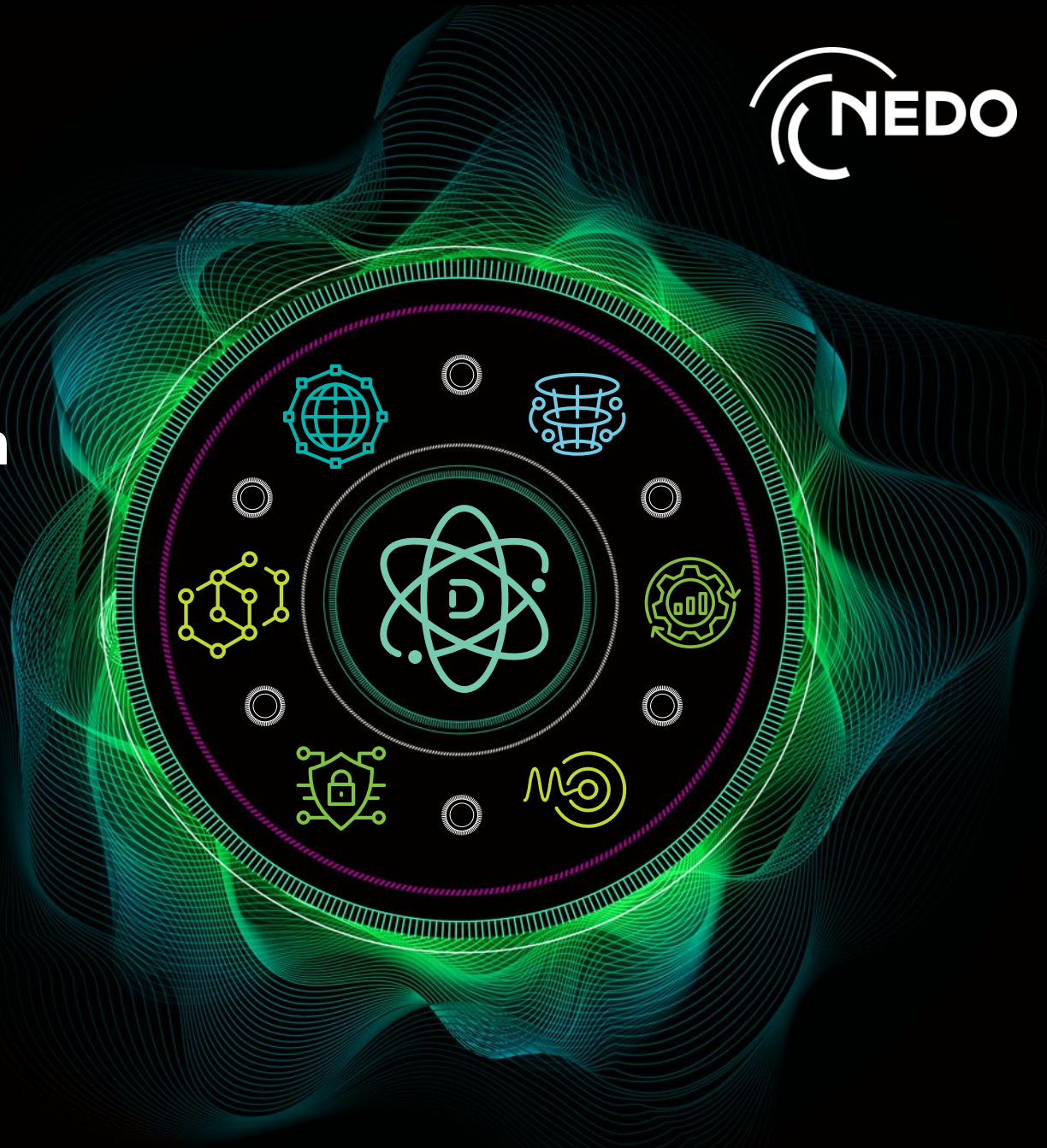
Quantum Computing Use Cases

Prediction of Allosteric Regulation of Proteins Expansion of drug discovery target

Revorf Toshiba Digital Solutions



New Energy and Industrial Technology Development Organization (NEDO)

Revorf Toshiba Digital Solutions: Prediction of Allosteric Regulation of Proteins Expansion of drug discovery target [2022/06] 1/2

Validation

Industry	Drug Discovery and Healthcare
Process	research and development
Method	combinatorial optimization
Category	Ising*

Background

- In the drug discovery process, **drug discovery target**, *1 and **exhaustion of drug discovery target** are issues.
- On the other hand, a drug discovery method focusing on allosteric control *2 (allosteric drug discovery) can find proteins that have been considered difficult to discover as drug discovery target candidates, and is expected to **solve the drug discovery problem of target depletion.**
- In order to discover the allosteric control site *3 in a protein, **in vitro experiments,** *4 and **computational alternative techniques** are required, which require a great deal of labor and time.

Issues and motivation to be solved

- **Quantum technology is expected to be used** to replace predictions of allosteric regulation of proteins with calculations rather than experiments
- In this verification, Revorf and Toshiba Digital Solutions jointly **developed a new technology to solve allosteric control prediction as a combinatorial optimization problem,** and **attempted to predict allosteric control sites by calculation,** which could not be specified by conventional calculation methods.

Expected business benefits

- By using this method utilizing quantum technology, **we succeeded in computationally predicting allosteric control sites that could not be identified by conventional methods**
  - ✓ Comparison of allosteric regulatory sites calculated and predicted by quantum technology with known allosteric regulatory sites for multiple proteins, including KRAS, an oncogene.
- This verification increased **the possibility of discovering allosteric control sites by calculation alone and accelerating the search for drug discovery candidate compounds**

*1: A protein that is assumed to be responsible for a disease and is targeted in the design of a drug.
*2: Mechanisms that specifically regulate the conformation and activity of proteins that provide functional diversity
*3: Regions of the protein other than the active center where regulatory molecules (allosteric factors) bind
*4: An experiment in which an environment that mimics in vivo is created artificially in a test tube or incubator.

Reference: Toshiba Digital Solutions Corporation "Utilizing SQBM+TM, a quantum-inspired optimization solution, to verify technology applied to computational drug discovery" (https://www.global.toshiba/jp/company/digitalsolution/news/2022/0627.html)
*Ising: A computing approach, mainly associated with quantum annealers and simulators specialized for the Ising model, in which a problem is first formulated as an Ising model and then solved computationally. It is particularly well suited to problems that involve finding the optimal combination from a vast number of possibilities.

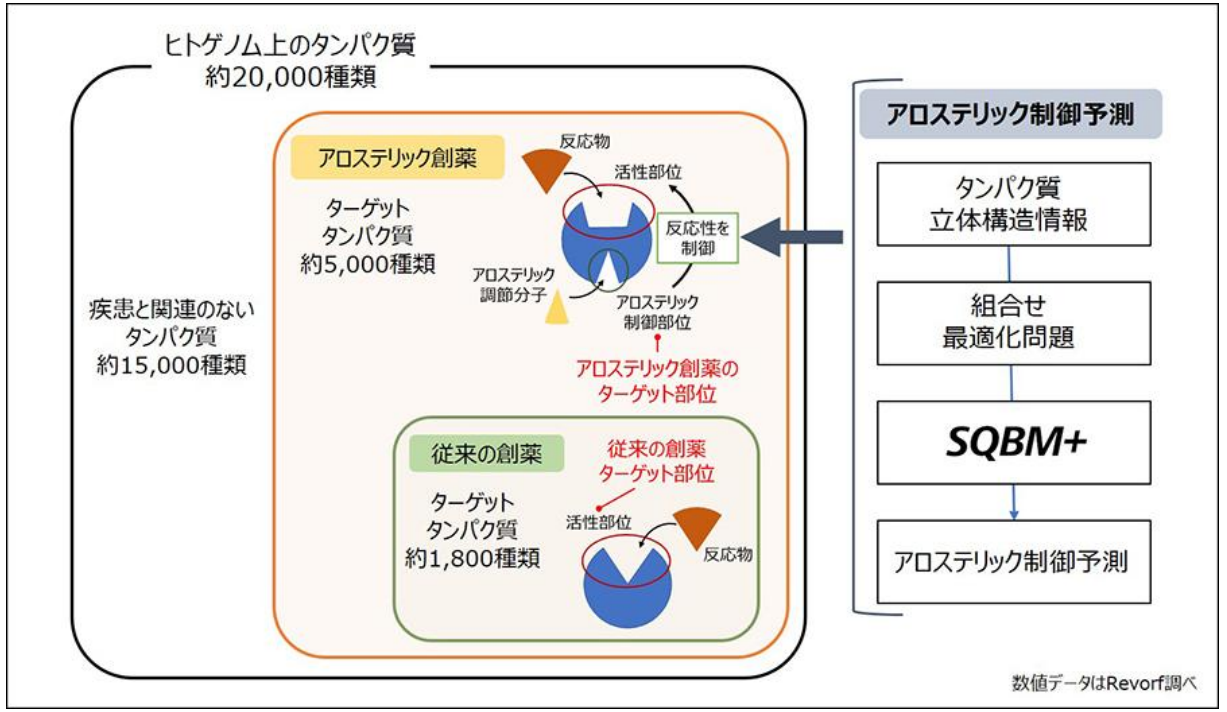
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Problem setting as a quantum computer

- In this verification, **the allosteric control mechanism of protein is formulated as a combinatorial optimization problem, and the allosteric control is predicted by calculation** based on the three-dimensional structure information of protein.
- The machine utilizes **SQBM +, Toshiba's quantum-inspired optimization solution**.



Reference: Toshiba Digital Solutions Corporation "Utilizing SQBM+TM, a quantum-inspired optimization solution, to verify technology applied to computational drug discovery" (https://www.global.toshiba/jp/company/digitalsolution/news/2022/0627.html)

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More use cases are available on our website. We invite you to explore them.
https://www.quantum-computing-use-cases.nedo.go.jp/english/

More Use Cases

New Energy and Industrial Technology Development Organization (NEDO)
AI and Robotics Department (e-mail: quantum_ai@ml.nedo.go.jp)

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