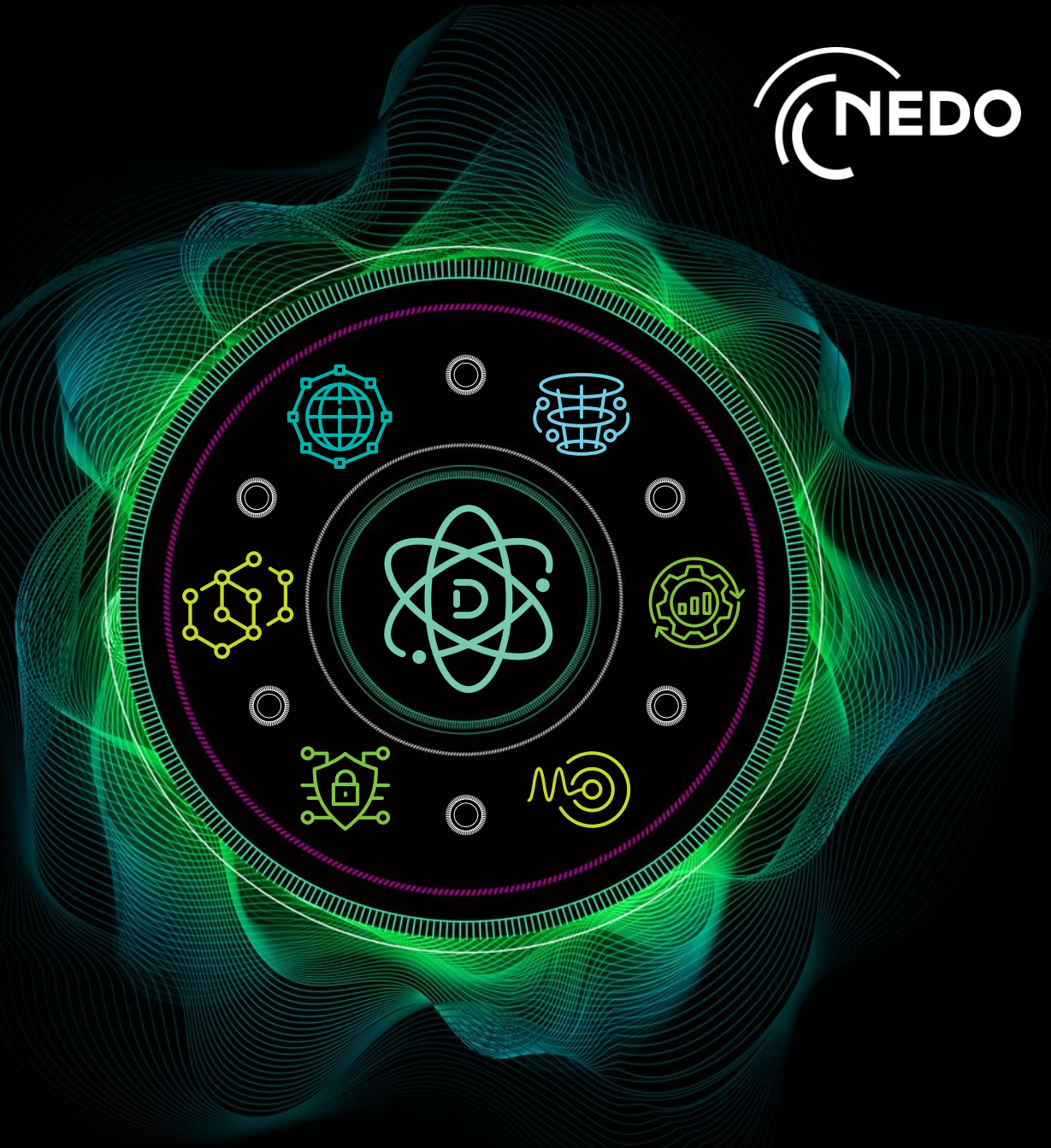
Quantum Computing Use Cases

Search for mid-molecule drug candidates

PeptiDream Fujitsu



New Energy and Industrial Technology Development Organization (NEDO)

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Validation

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

Background

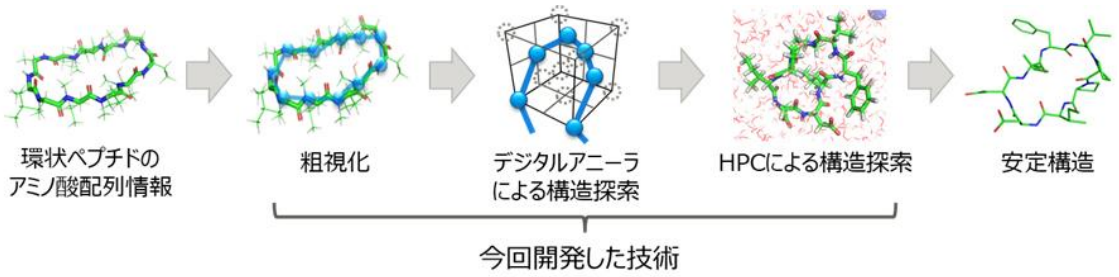
- PeptiDream is **developing a number of mid-molecule drug candidates.**
  - ✓ Medium-Molecule drugs are attracting attention because their molecular weight is between that of small-molecule drugs and antibody drugs (macromolecules), and because they combine the advantages of relatively low cost and low side effects.
- In the development of drug candidate compounds, **in the process of narrowing down candidate compounds from a library of several trillion compounds, it is difficult to search stable structures with conventional computers, and development takes a considerable amount of time.**

Issues and motivation to be solved

- Because **it is difficult to search for stable structures with classical computers and wet experiments must be repeated,** medium-molecule candidates **typically take months to years.**
- To solve this problem, Fujitsu and PeptiDream have started a joint research project to **develop a new basic technology to search the stable structure of medium-sized cyclic peptides as candidate compounds for drug discovery at high speed and with high accuracy** by utilizing quantum technology.

Problem setting as a quantum computer

- **Quantum and classical computer techniques were applied to search for stable structures of medium-sized cyclic peptides.**
  - ✓ Development of **Technology to Search for Stable Structures of Medium Molecules Using Coarse-Grained Structures** to Calculate Complex Molecular Structures Fast and Efficient Using Quantum Technology
  - ✓ **Development of technology to automatically convert coarse-grained models of candidate compounds obtained by quantum technology into all-atom models (models representing molecular structures using all atomic coordinates)**
- We use **Fujitsu digital annealer** as a quantum computer technology.



Flow of Search for Stable Structures of Medium-Sized Cyclic Peptides

Reference: Fujitsu Limited "Fujitsu and PeptiDream Search for Medium-Molecule Drug Candidates Fast, Accurately" (https://pr.fujitsu.com/jp/news/2020/10/13.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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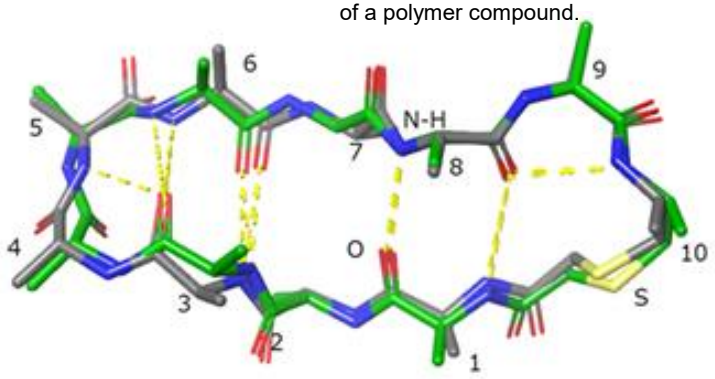
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Expected business benefits

- **Using the newly developed technology, we succeeded in performing a high-speed search for the stable structure of a medium-sized cyclic peptide with high accuracy within 12 hours,** which was considered difficult to obtain by conventional classical computer calculations
- Comparing the structures calculated by the newly developed technology with those derived from actual experiments, **the possibility of searching for candidate compounds that are almost the same as those in actual experiments with high precision and minimizing the experimental steps required to search for candidate compounds** has been raised.
  - ✓ The deviation of the main chain * is 0.73 angstroms (1 angstrom =0.1 nanometers), which is as accurate as the experiment.
- By shortening the research period and the experimental period, it is possible to use the remaining time to develop new drugs.

*: Molecular chains that form the backbone of the structure of a polymer compound.



Comparison of experimental and computational structures
(Only the main chain is shown; gray is the experimental structure; green is the calculated structure.)

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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

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This collection of use cases was obtained as a result of the work commissioned by the New Energy and Industrial Technology Development Organization (NEDO) "Cyber-Physical Development Business of Quantum/Classical Hybrid Technology/Study of Use Case of Quantum Technology" and the “Post-5G Information and Communications System Infrastructure Reinforcement R & D Project (Quantum Industrialization)/Comprehensive Study for Promoting the Industrialization of Quantum Computers”.