Quantum Computing Use Cases

Development of a Large-Scale Virtual Screening Method for Drug Discovery Using a Quantum–AI Hybrid Approach

Toshiba Digital Solutions, Ahead Bio Computing, and Institute of Science Tokyo



New Energy and Industrial Technology Development Organization (NEDO)

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Validation

Industry	Drug Discovery and Healthcare
Process	lead search and optimization
Method	combinatorial optimization
Category	Ising*

Background

- In hit compound identification at the early stage of drug discovery, **virtual screening (VS)** is used to computationally select compounds from many candidates that are expected to bind to a target protein and serve as starting points for drug discovery
- In recent years, virtual compound generation using generative AI and related methods has expanded the number of candidate compounds to the order of 10^9 or more. Meanwhile, conventional VS methods evaluate each candidate compound sequentially, so **computation time, resources, and cost increase in proportion to the number of candidates**
- As a result, VS that fully leverages vast candidate compound data tends to be limited to a small number of companies and research institutions that can secure large-scale computing resources. For pharmaceutical companies, **balancing broader search space with computational cost has become a major challenge**
- **This creates a need for a new large-scale VS method that can process a vast number of candidate compounds within practical time and cost constraints**

Issues to be solved and motivation

- The goal is to **develop a method that significantly reduces computation time for a vast number of candidates while maintaining accuracy comparable to conventional VS methods**
  - ✓ This would reduce the cost of VS and improve the efficiency of the drug discovery process
- In this effort, **compounds are treated as combinations of fragments, which are their substructures, and VS is formulated as a combinatorial optimization problem**
- Because the number of fragment types included in the candidate compounds is far smaller than the number of candidate compounds, **promising candidates can be narrowed down by searching for good combinations of fragment placements, without directly evaluating the entire compound space**
- In addition, the quantum-inspired optimization solutions SQBM+ used as the combinatorial optimization solver can rapidly output many near-optimal solutions, that is, diverse candidates close to the optimum. This makes it suitable for VS, where multiple diverse candidate compounds are needed rather than a single optimal solution

Reference: AI and Robot Department, New Energy and Industrial Technology Development Organization (NEDO), "Cyber-Physical Development Project for Quantum-Classical Hybrid Technologies" (https://www.nedo.go.jp/content/800030349.pdf); Toshiba, "SQBM+, Quantum-Inspired Optimization Solutions" (https://www.global.toshiba/jp/products-solutions/ai-iot/sbm.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.

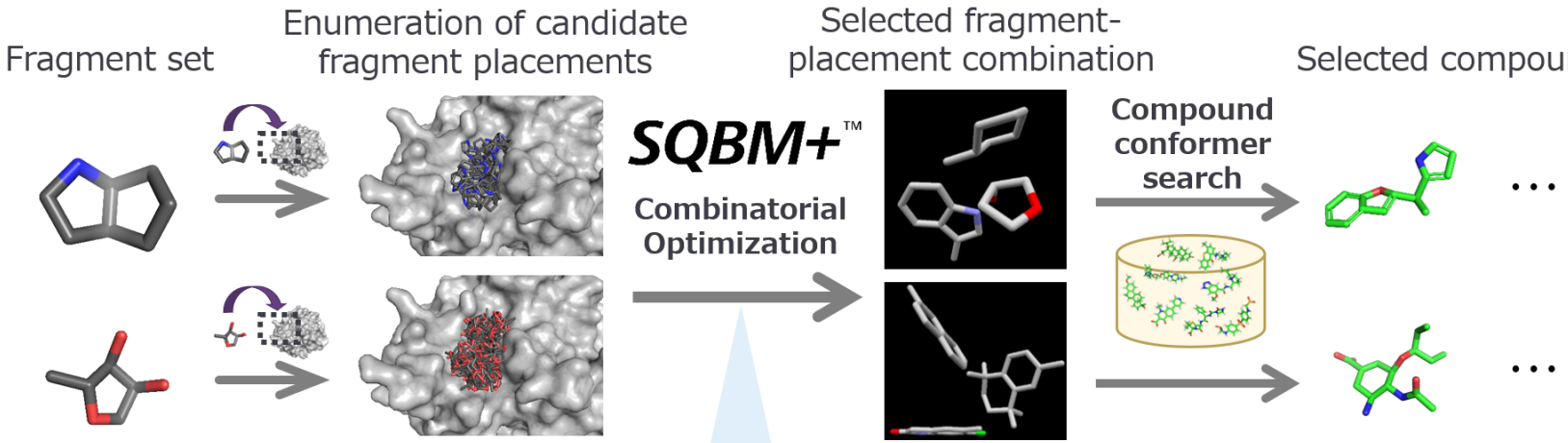
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Problem formulation for quantum computers

- VS was **formulated as a problem of selecting combinations that are chemically plausible and expected to bind, from a large number of candidate fragment placements enumerated** around the binding pocket of the target protein, where the drug compound binds and exerts its effect
- **A new method, Frasco-VS, was developed to rapidly narrow down promising compounds** by searching a compound library for compounds similar to these combinations



Processing flow of Frasco-VS

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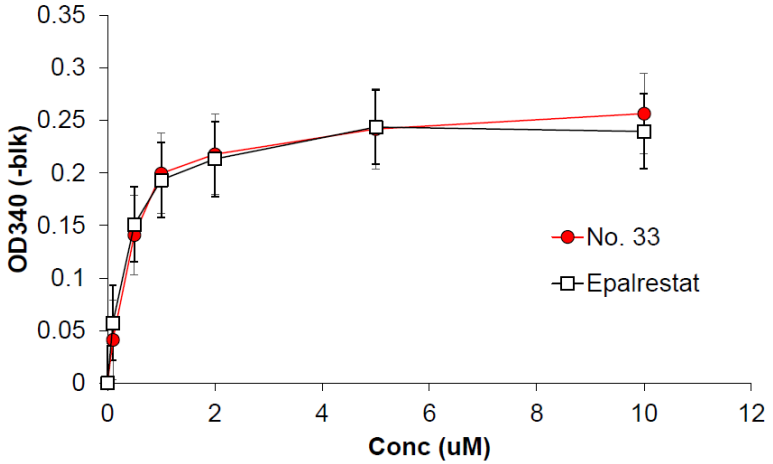
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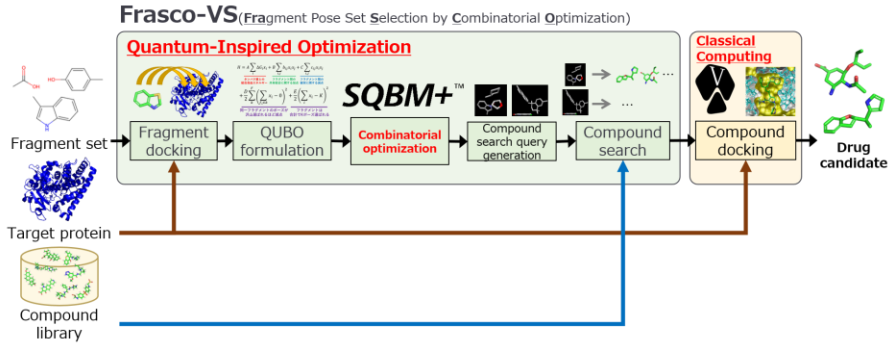
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Expected business benefits

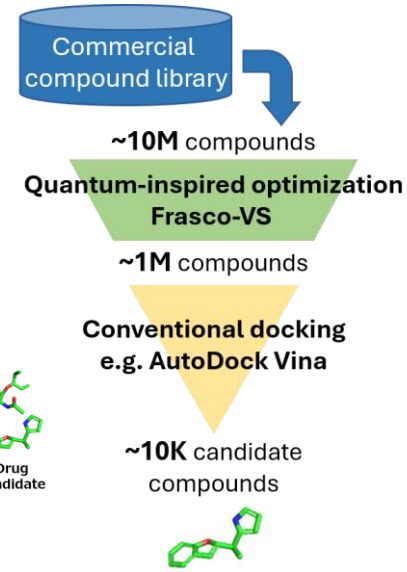
- Shorter hit identification time and lower cost in the early stage of drug discovery. The larger the target compound library, the greater the advantage over conventional methods
- In a demonstration targeting aldose reductase (ALDR), a protein related to diabetes, **the method was about 10x faster than the conventional approach. An *in vitro* study also identified one novel compound with inhibitory activity comparable to the existing drug epalrestat**, confirming the effectiveness of the proposed method
- The approach is hybrid: Frasco-VS first narrows down candidate compounds broadly, and classical computation in the second stage applies stricter screening
- The system has already been built to run on AWS, a general-purpose cloud environment, and on ABCI-Q of the National Institute of Advanced Industrial Science and Technology. This enables companies and research institutions without their own large-scale servers to carry out VS on a vast number of candidate compounds



Novel ALDR inhibitor discovered using the proposed method



Configuration of the hybrid method combining Frasco-VS and classical computation



Reference: AI and Robot Department, New Energy and Industrial Technology Development Organization (NEDO), "Cyber-Physical Development Project for Quantum-Classical Hybrid Technologies" (https://www.nedo.go.jp/content/800030349.pdf); National Institute of Advanced Industrial Science and Technology (AIST), G-QuAT, "ABCI-Q: Quantum-Classical Hybrid Computing Platform" (https://unit.aist.go.jp/g-quat/HowToUse/abci_q/index.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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