Fujitsu
uvance

FUJITSU

Accelerating drug discovery with AI, Quantum, and High-Performance Computing

Advanced technologies transforming drug discovery

The landscape of drug discovery is on the verge of a revolution, powered by new technologies such as artificial intelligence (AI), quantum computing and high-performance computing. The traditional wet labs approach, centered on in vitro experiments, is being augmented with digital laboratories, which can leverage these advanced technologies to perform experiments in silico.

With this paradigm shift, the roles of chemists and biologists are expanding, as they begin to collaborate with computational chemists, who are adept at navigating these emerging technologies. They bring unique skill sets and value, thereby necessitating an increased investment in these cutting-edge technologies and personnel over the forthcoming decade.

However, the optimal investment in new technologies, and the people who can leverage them, is far from clear. Where can research organizations get the best return on investment? Which technology is appropriate for which problem? Or perhaps a mix of technologies is best? Which technologies are mature enough to put to practical use? How should my research organization invest to stay on top of these new developments and remain competitive? How much should technology be developed in-house versus leveraging partners? Which partner has the competencies and experience to ensure my organization's success?

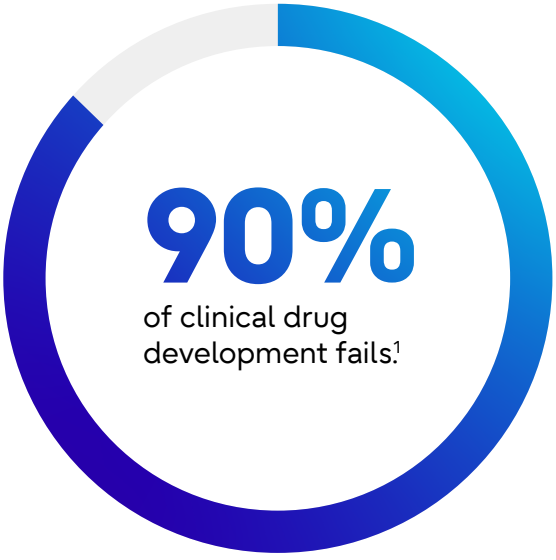
Drug discovery leaders and executives should be forgiven for being overwhelmed by all these questions and feeling a bit in the dark. This white paper sheds light on these challenges by sharing how Fujitsu has successfully deployed AI, quantum computing and high-performance computing to address challenges in drug discovery, working in collaboration with industry partners.

Recognizing the risks of early-stage drug discovery

Early-stage drug discovery requires a multi-year commitment to designing, testing and validating new drug combinations before being able to advance to production. Should a hypothesis be invalidated, the cycle must start anew.

This low probability of success can be disheartening for the researchers who dedicate large portions of their careers to driving forward the collective understanding of diseases. Pharma decision makers tend to be acutely aware of opportunity cost of allocating resources – both time and personnel – towards a project that might not make it to market.

Caution also exists around the safety risks of progressing with new drug combinations that may have unknown side effects, not to mention the regulatory and legal risks of pursuing drugs that are ultimately deemed unsafe.



Matching the innovation cycle with investment

While investment has been a tailwind for the sector in recent years, the low probability of success can also hold back discovery and development processes that might lead to groundbreaking discoveries.

On average, bringing a new drug to market can be a 12 year-plus endeavor[2]

of which roughly five years are associated with early-stage drug discovery. The process typically requires in excess of $2 billion in investment over the entire development cycle.[3]

Investors involved in early-stage pharma tend to have deep specialization in the sector and understand the financial risks of undertaking multi-year development. While this risk-reward dynamic is typically factored into their decision-making from the outset, they will still want to see proof of value as early as possible in order to project the likelihood of returns.

Technological innovation can help to counteract the opportunity cost associated with these investments. For example, AI tools are helping to shorten the conventional cycle necessary to identify preclinical candidates from five years to just 12 to 18 months, inclusive of synthesis and in vitro testing.[4]

[1] ScienceDirect
[2] Cancer Research UK
[3] Policy & Medicine
[4] BCG

Racing towards the quantum age: The benefits of including a quantum computing approach

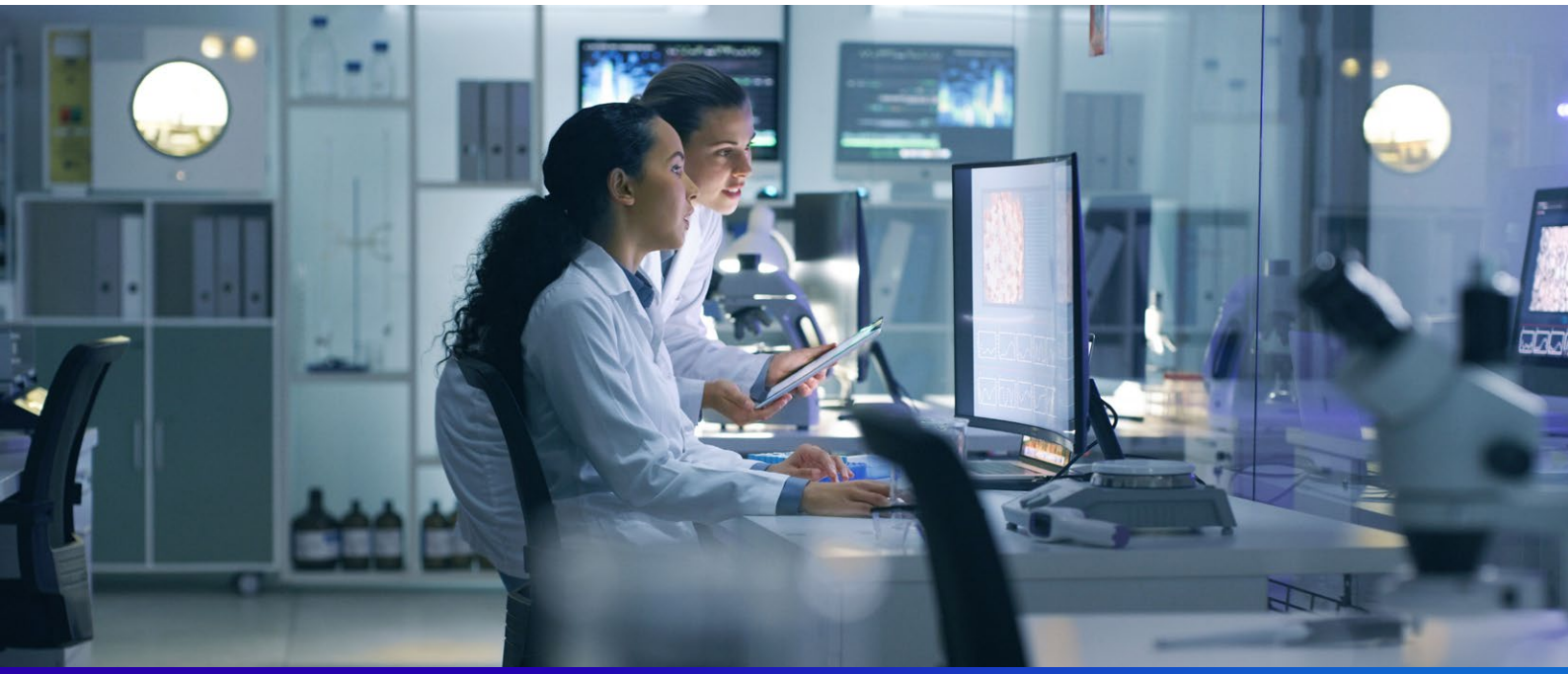
Given the advantages enabled by new computational technologies, drug discoverers are investigating what options can support and enhance the exploration processes. An essential preliminary decision revolves around where and when to deploy AI or more computationally intensive techniques such as quantum computing. While these are complementary approaches, the choice of which to use in specific cases and phases will depend on the scale of the data being processed as part of their study.

The use of AI in drug discovery is steadily gaining recognition, and has proven effective for certain tasks. AI applies machine-driven automation to available data sets to perform research tasks which traditionally would have relied on human knowledge. AI certainly has its place and can have a significant impact on the efficiency of drug discovery, helping to improve accuracy and efficiency.

Only quantum computing, on the other hand, provides the computational power to evaluate libraries with billions of molecules. Quantum algorithms effectively evaluate and reduce this vast universe, eliminating unviable candidates and narrowing the search space, resulting in a dramatic increase in efficiency.

This approach also improves the efficiency of the 'wet chemistry' lab by ensuring that only those molecules with a high probability of success proceed to this stage. As a result, the process saves precious resources that would have been expended in synthesizing and testing molecules that have a high probability of failure.

Using a quantum-inspired approach, therefore, researchers can experience 'failure' earlier on in the process, before the pre-clinical and clinical stages. This process of invalidation allows them to avoid potential dead ends and only progress with drug combinations that demonstrate higher likelihoods of success.



Convergence of cognitive advanced technologies

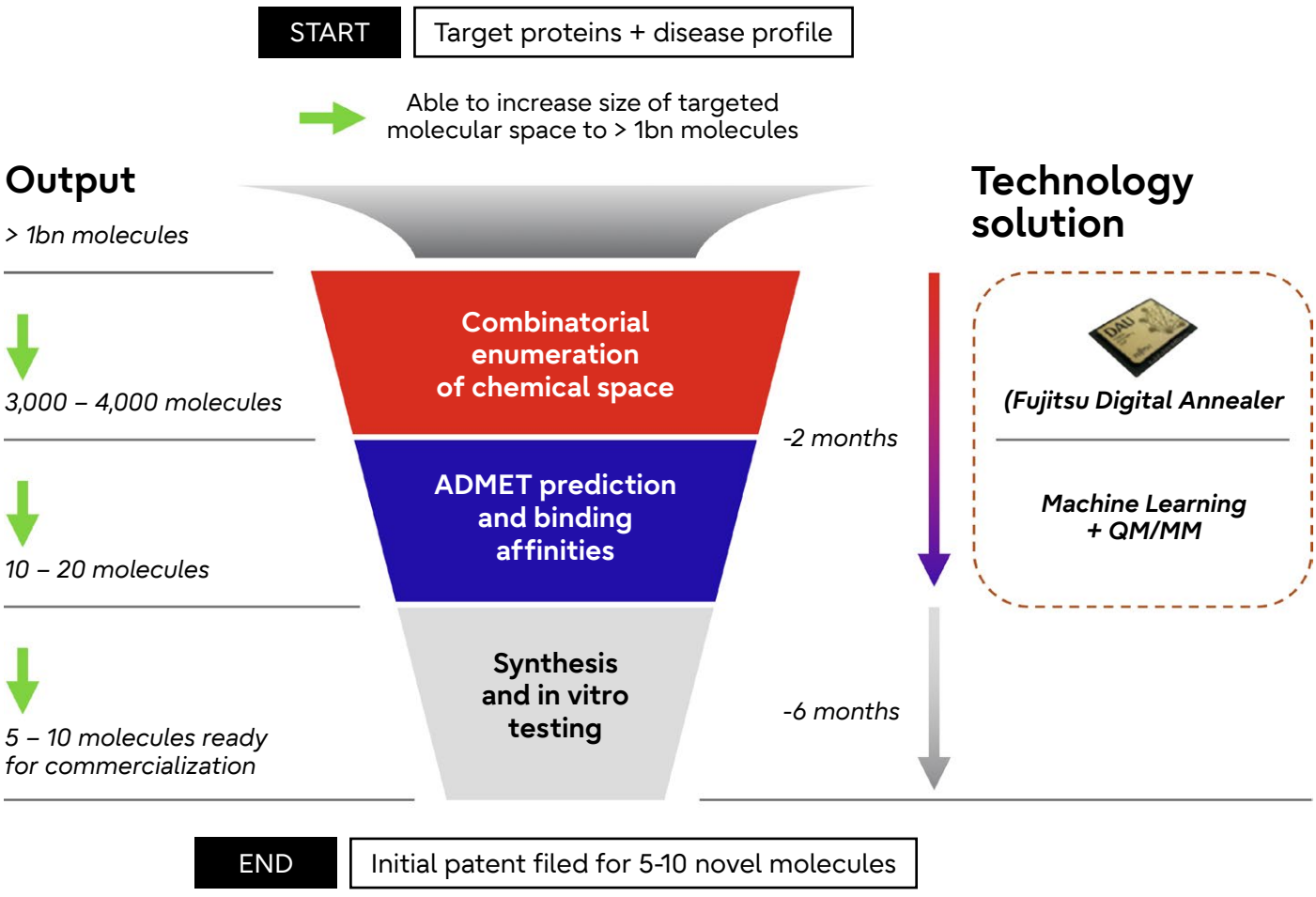
While AI and quantum-computing approaches offer differing functionality, they can also be employed in unison as part of a holistic approach.

Significant strides have been made in AI-based drug discovery, particularly in the area of rapid estimation of the chemical properties of molecules. Quantum and quantum-inspired add a new dimension of capability, with the key attributes of computational speed for problems with exponential size.

In scenarios where the approaches can be combined, AI can complement a quantum approach for rapid estimation of chemical properties for further refinement, such as ADMET properties, once the search space has been significantly narrowed using quantum techniques.

The addition of a quantum approach to an AI platform can also create a diverse set of target molecules during initial lead generation, thereby enhancing the likelihood of finding therapeutic molecules.

It is important for decision makers to see these technologies as convergent and complementary, as opposed to exclusive, as the potential impact can far outweigh that of any single approach.



Supporting early-stage drug discovery with advanced computational solutions

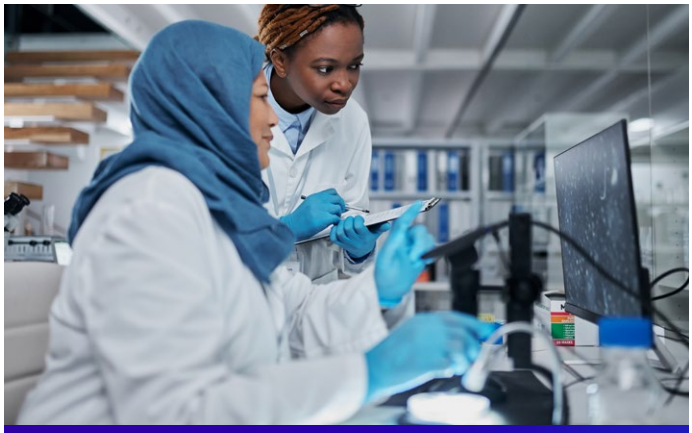
Fujitsu Digital Annealer

Fujitsu's Digital Annealer (DA) is a pre-quantum special-purpose technology designed to solve large combinatorial optimization problems. It is presently being applied to drug discovery, enabling the identification of promising molecules from massive data sets.

The DA drug discovery solution focuses on early-stage discovery of small molecules. The solution enumerates a library consisting of billions of candidate molecules which can be rapidly assessed at a scale not possible with AI technologies. Based on their findings, researchers then have the opportunity to reformulate and retest hypotheses to increase the pace of finding promising results.

The solution offers higher volume capabilities than a solely AI-based approach and is able to return results in less than a month. Using the DA, researchers can apply quantum techniques now and bridge to future quantum technologies as they become more mature.

Pharma companies will also find that the DA potentially has applications in their business beyond just drug discovery. For example, the solution can be applied to combinatorial optimization problems across the supply chain and manufacturing cycle, creating further efficiencies and economies of scale.



Co-creating advanced discovery capabilities

POLARIS^{qb}, a drug research company, worked with Fujitsu to create drug blueprints ('leads') for inhibitors of Dengue Fever RNA-dependent RNA polymerase enzyme, which plays a crucial role in infection from the virus.

Together we co-created a drug discovery platform based on a combination of quantum-inspired computing, AI, and precision medicine to research the chemical space to create novel molecular drugs for specific proteins and diseases.

Using the Digital Annealer drug discovery solution, POLARIS^{qb} was able to dramatically speed up the drug discovery process.

The solution helped to cut hit identification and hit-to-lead optimization timelines from 48 months down to just eight.

Fujitsu High Performance Computing (HPC)

Fujitsu is pioneering advances in supercomputing through the Fugaku petascale supercomputer.

For example, Fujitsu has launched a joint project with Riken, a scientific research institute based in Japan, on next-generation IT drug discovery technology, utilizing Fugaku. The use of HPC to explore small molecule targets creates the potential to dramatically reduce the development period and costs for new drugs, as well as the scalability needed to meet increasing performance demands of the future.

The technology is expected to be developed by the end of 2026.

Applying HPC and DA to enable high-precision drug exploration

PeptiDream is a leader in proprietary technologies for peptide drug discovery. Fujitsu collaborated with PeptiDream on a joint research project that involved application of quantum technologies to cyclic peptide drug discovery, narrowing down several trillions of libraries to find stable confirmations and streamline the drug discovery process.

Together, Fujitsu and PeptiDream combined DA with HPC to create a technology platform to improve the search process for candidate compounds. The platform enabled high-speed and high-accuracy conformational search for peptides, and helped to overcome issues with data accuracy in peptide research.

Going forward, this research and platform will enable the discovery and development of new drugs previously considered impossible due to time and cost constraints.

Driving progress for drug discovery

It's crucial for research organizations to map out their journey towards digital drug discovery, incorporating advanced technologies into their processes. Fujitsu is leading in this space through solutions which leverage AI, HPC, quantum computing, and more. Together, we can maximize the impact of these new technologies on your research team's transformation, enabling rapid and efficient results.

Collaborative innovation

Partner with industry experts to pinpoint problems and unlock value from the get-go, harnessing the synergy of advanced and quantum-inspired technologies.

Expert consultancy and tailored solutions

Leverage our global expertise in digital solutions to tackle complex business challenges. Grasp the full potential of next-generation computing and prepare for tomorrow by optimizing drug discovery processes and coding in QUBOs.

Rapid value realization

Experience heightened simulation accuracy in early-stage clinical trials, powered by advanced computational solutions, leading to increased predictability and returns on investment.

Minimized risk

Embrace a 'fail fast' mentality, driven by AI insights and DA's capabilities, to mitigate financial risks and avoid squandering resources on fruitless endeavors.

Ready for future tech

Harness the power of exciting new technology today, and as it continues to evolve. Our trailblazing solutions can help you make the most of all the extraordinary possibilities the upcoming decade holds.

Get ready to leap into the future of drug discovery with Fujitsu – where cognitive and cutting-edge technologies converge to reveal a world of possibilities.

To start your drug discovery digital transformation journey visit **our website**

Or email us at:
drugdiscovery@fujitsu.com

Fujitsu uvance

FUJITSU

FUJITSU-PUBLIC