De Novo Digital Drug Design Platform

A new quantum-inspired platform that brings together pioneering technology from Fujitsu and Polaris[qb] to significantly improve the speed and chemical diversity of small molecule lead discovery, tested on the Dengue Fever polymerase.

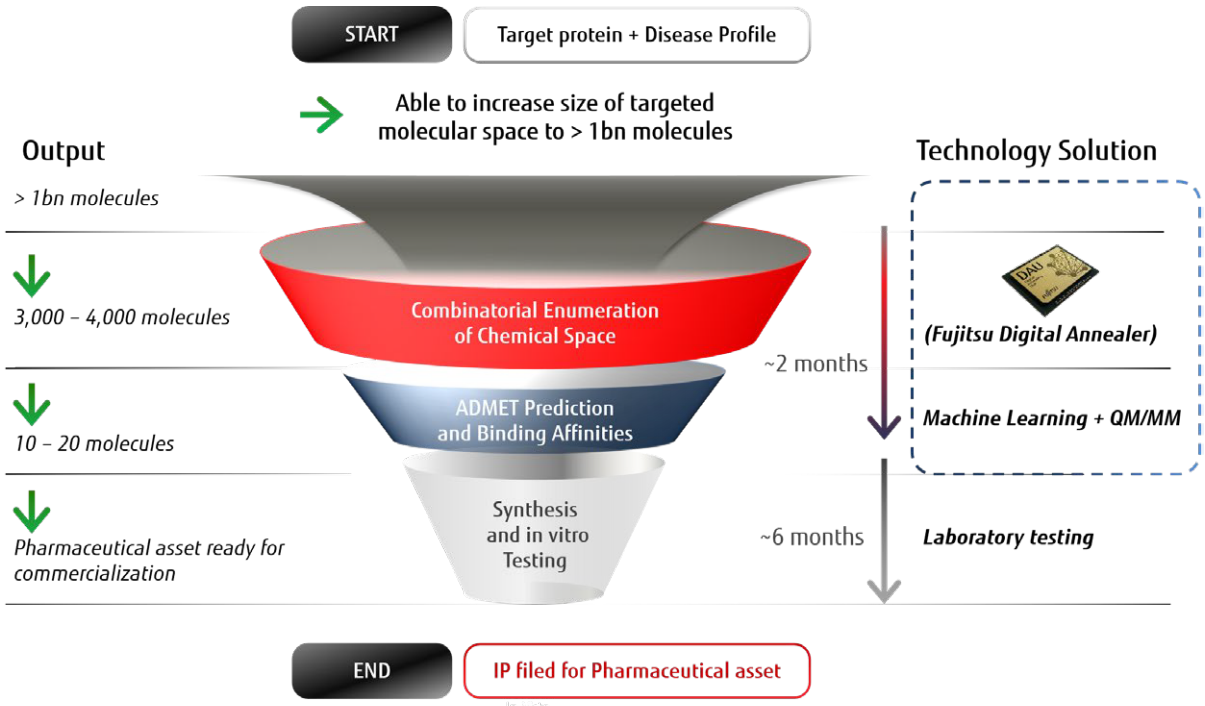
Platform Overview

A novel solution combining quantum-inspired technology, machine learning and Quantum Mechanics / Molecular Mechanics (QM/MM) simulations improving both speed and chemical diversity in designing novel lead candidates. This will significantly impact early stage drug discovery by reducing typical timelines from 24-48 months to approximately 8 months. Molecules will be taken straight to in vitro testing without cycling through the usual drug modelling/in vitro research loop.

Additionally, the quality of leads is improved by screening a far larger targeted chemical space of over 1 billion molecules. The outcomes will be patentable, novel molecules that have optimized drug-like qualities, low toxicity, synthesizability, and are biologically active.

The Platform

The platform identifies lead molecules candidates from a targeted, large and diverse virtual library of several billion molecules and assesses their quality. Leads are evaluated using the structural information of the pharmaceutical target and a set of physicochemical constraints, such as Absorption, Distribution, Metabolism, Excretion and Toxicity (ADMET) etc. The platform leverages an annealing based molecule filter harnessing the computing power of Fujitsu's Quantum Inspired Technology. The output is then refined and ranked with Polaris[qb] machine learning algorithms for physicochemical properties, and QM/MM simulations for binding affinities. The final output is a short-list of high-quality molecules prioritized for synthesis and in vitro testing.



The Technology Powering the Platform

Fujitsu's Digital Annealer: The quantum-inspired Digital Annealer solves combinatorial optimization problems 10,000x faster than any other currently available alternatives. It is based on custom hardware, is production ready and is accessible as a cloud service as well as on-premises. Forward looking customers are using the Digital Annealer to future proof their computational strategy for the Quantum Revolution. A repeatable approach to molecule optimization is possible through an annealing based molecule filter executed on the Digital Annealer.

Polaris[qb] QMD Drug Design Platform: Polaris, an RTP-based start-up and Cloud Pharmaceuticals' spin-out, uses Machine Learning combined with QM/MM simulations to design small molecule drug leads. These leads have strong binding affinities and desirable drug properties for a specific target and therapeutic profile. Previously, Quantum Molecular Design (QMD) designed active lead molecules for Dengue, Sepsis and Crohn's Disease.

Through co-creation, we are developing a novel hardware-software best-in-class drug design solution. Our early validation target is a previously un-drugged Dengue virus protein. A short-list of high-quality molecules for this protein will be available to partners to take through to the next stage by May 2020.

Dengue virus as a Proof of concept

Though Dengue Fever outbreaks are a recurrent theme in most tropical countries with ~100 million affected every year, the 1st case of Dengue contracted in the United States was discovered in Miami in 2019, and based on predicted climate changes, the mosquito vector of Dengue is moving toward unprotected populations. We have used our technology to study the Dengue RNA-dependent RNA polymerase protein, and optimize novel inhibitors, with the aim of treating Dengue in both developed and developing countries.

The Value for Drug Discovery

- Quality – Our platform expands the size of the searchable chemical space from 0.5 – 10 million molecules (market standard) to billions of molecules, thereby increasing the likelihood of finding novel, viable drug candidates.
- Speed – This approach significantly reduces the total time to find de novo drug leads from a historical 24-48 months to approximately 8 months by accelerating the molecular design and refinement process.
- Scalability – The platform is designed to perform rapid virtual screening of large (>1bn molecules) molecular libraries to support lead discovery.

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