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Harnessing the power of quantum computing for drug discovery

POLARIS^{qb} is slashing the timeframes and costs of drug discovery by using the unique processing power of quantum technology to identify the best lead compounds for drug development.

Traditional computer-aided drug design (CADD) helps researchers screen for potential new drug-like molecules and predict their biological activity before completing laboratory experiments. However, for most systems, it takes too long to explore all possible compounds with drug-like characteristics, so searches are constrained to a relatively small pool.

CADD is an iterative process requiring a series of optimizations. "Once you find a molecule which binds to your target, you optimize it to bind better, be more soluble, be more stable, less toxic, etc." Shahar Keinan, CEO of Polaris Quantum Biotech (POLARIS^{qb}), explained. "By starting from a much larger chemical space and transforming drug design to an optimization problem, we can find molecules with all the requisite properties in a single step".

Keinan and Bill Shipman, Chief Technology Officer of POLARIS^{qb}, have been working towards this objective since co-founding the company in 2020. "With our quantum-inspired technology, we can efficiently scan large chemical spaces for potential drugs at unparalleled speed," Keinan said.

POLARIS^{qb} built the first drug discovery platform that uses a quantum annealer, a specialized type of quantum computer that solves combinatorial optimization problems. By leveraging the principles of quantum physics, a quantum annealer can quickly solve very complex multi-object optimization problems that are prohibitively difficult for classical computers.

"Rather than using a brute-force approach to calculate all possibilities, the wave function of a quantum system scans all possibilities to find the best molecule out of billions the first time," said Keinan.

POLARIS^{qb} specializes in translating chemistry into the language of quantum computers. "We know how to create chemical space in the format of quadratic unconstrained binary optimization (QUBO) algorithms[1] that run on a quantum annealer for optimization," she said.

A validated approach

POLARIS^{qb} is working on over 15 drug discovery projects and building a promising portfolio of lead molecules.

To demonstrate the validity of the approach, computational chemists at POLARIS^{qb} identified drug candidates that target the RNA-dependent RNA polymerase of the Dengue virus, a mosquito-borne viral disease that currently has no cure and threatens up to 40% of the world's population[2]. The team built a chemical library of 1.3 billion compounds and used a quantum annealer to assess the library and to design molecular leads. Within six months they were able to prioritize molecules for experimental testing. Out of 30 final lead molecules, 10 shared similar motifs with molecules that are active in cells identified after seven years of effort by Novartis[3].

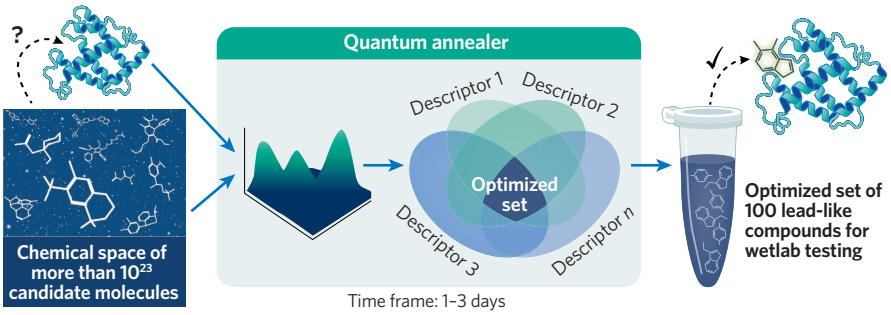

Fig. 1 | The QuADD platform. Identifying a top enriched library of candidates in days.

Working with POLARIS^{qb}

POLARIS^{qb} has partnerships with several companies seeking to integrate quantum technologies and advanced artificial intelligence (AI) to discover novel lead compounds for a wide range of medical indications.

POLARIS^{qb} is working with Auransa to find therapeutics for diseases that disproportionately affect women. By combining their expertise in AI-driven biology and quantum-computing-based chemistry, they are searching and testing molecules that target a dysregulated pathway in triple-negative breast tumors.

"We are delighted with the progress we are making with POLARIS^{qb} and are continuing to tackle complex women's diseases and bring much-needed therapeutics into the clinic," said Pek Lum, CEO of Auransa.

POLARIS^{qb} is a service provider to companies developing small drug-like molecules against specific targets. POLARIS^{qb} builds and searches large chemical spaces based on the client's criteria. "We are often approached to find drug-like molecules against difficult targets, such as G protein-coupled receptors (GPCRs) or protein–protein interactions (PPIs)," Keinan said. "We are very good at finding molecules that are hydrophobic enough to bind pockets in PPIs but soluble enough to reach them."

POLARIS^{qb} can recommend ~100 lead molecules with the desired biological activity and properties, including synthesizability, within 3 to 4 months.

At the end of June 2023, POLARIS^{qb} will also be offering a Software-as-a-Service (SaaS) platform called QuADD that is executed on a quantum annealing system. Customers will be able to submit their target and small-molecule requirements to the QuADD platform, which will scan across a large chemical space while maintaining data confidentiality (Fig. 1).

Out of many billions of molecules, POLARIS^{qb} identifies the top enriched library of candidates in a matter of days. Customers can load these results into their proprietary CADD workflow, use their internal algorithms to further optimize the QuADD results, and speed up the hit-to-lead process. Proof-of-concept testing established that QuADD successfully reverse-engineered known drugs. For example, starting from the human P38 mitogen-activated protein (MAP) kinase protein-binding pocket, QuADD suggested a set of fragments that corresponded to Nexavar (sorafenib), a commercial oncology drug.

"To my knowledge, this is one of the first SaaS quantum-based products available on the global market and the only one for drug design," said Keinan. "It's increasingly difficult to find new lead molecules, but using QuADD to create novel, enriched molecular libraries of lead molecules will close this discovery gap.

1. Maurice Benson, B. et al. Preprint at *arXiv* https://arxiv.org/abs/2303.15419 (2023).
2. Whitehorn, J. & Simmons, C. P. *Vaccine* **29**, 7221–7228 (2011).
3. Snelling, D. et al. Preprint at *ChemRxiv* https://doi.org/10.26434/chemrxiv.12229232.v2 (2020).

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