

POLARIS^{qb}

Launching Tachyon™, the world's first drug discovery software built for quantum computing, to shorten years-long preclinical drug design and optimization process to a few months

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Founded in 2020
Co-Founder & CEO: Shahar Keinan, Ph.D.
No. of employees: 13
Type of Ownership: Private
Primary stock exchange: N/A

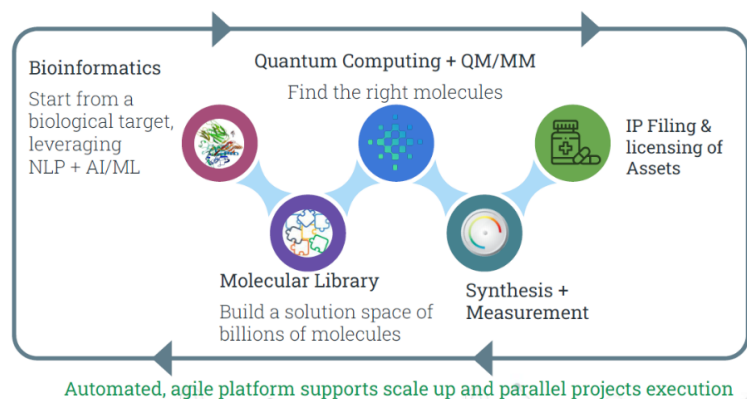
May 2022: Leveraging quantum computing, cloud, and AI to identify early stage drug discovery solutions 10,000 times faster than any existing solution in the market.



Venture Valuation (VV) interviewed Shahar Keinan, Ph.D, Co-Founder and CEO.

- VV:** By combining physics, biology, and chemistry together, your proprietary Tachyon™ quantum computing platform is able to narrow the field of candidate molecules from the billions down to dozens of potential leads in a short time.
- Keinan:** The significant advantage of Tachyon™ is the automation of the software capable of utilizing a quantum computer to optimize multiple molecules in much faster runs than existing computing solutions. Simultaneously Tachyon™ supports scale up and executes multiple parallel projects. The image below shows the workflow.

Tachyon: POLARIS^{qb} Drug Design Platform



With machine learning algorithms on internally curated data from previous runs, each run updates internal models. Consequently, the more projects are completed, the more powerful Tachyon™ becomes.

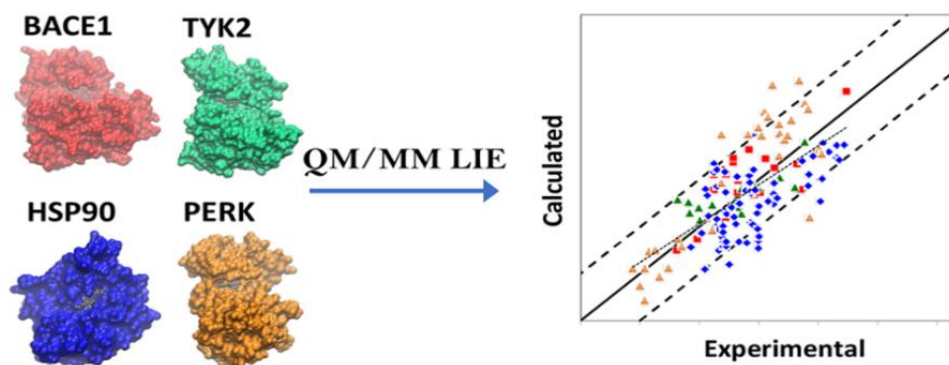
By using D-Wave quantum annealer (5,000 qubits), Tachyon™ assesses a huge chemical space at once. Theoretically, chemical space is estimated to be 10^{65} small molecules. This enormous space contains every molecule that has ever been synthesized, or will be synthesized in the future, including all current and future molecular drugs.

Currently Tachyon™ manages a library of over 4 billion molecules, identifies the correct molecule or molecules based on a number of targeting and drug like properties, and creates customized libraries for each target and disease profile.

VV: Along with quantum computing you are applying QM/MM (Quantum Mechanics/Molecular Mechanics) simulation method to increase accuracy and speed as well as LIE (Linear Interaction Energy) to evaluate the binding affinity.
Keinan: QM/MM is a multi-scale/multi-resolution computational chemistry method that treats different parts of the systems with different levels of calculations.

QM/MM was presented by Arieh Warshel and Michael Levitt in their 1976 paper “The development of multiscale models for complex chemical systems”. They won the 2013 Nobel Prize in Chemistry together with Martin Karplus.¹

The graph below is from the article published in The Journal of Physical Chemistry². It shows QM/MM +LIE calculated binding energy (kcal/mol) versus experimental binding energy (kcal/mol) for BACE1 (red square), HSP90 (blue diamond), TYK2 (green triangle), and PERK (orange triangle).



These four proteins are selected based on diversity of protein type, the availability of X-ray structural data with bound inhibitors, and experimental binding affinity data.

QM/MM + LIE method has demonstrated an 80% accuracy and precision rate in predicting binding affinity. Furthermore, none of the extensive costs of other

¹ <https://www.nobelprize.org/prizes/chemistry/2013/summary>

² In Silico Prediction of Ligand Binding Energies in Multiple Therapeutic Targets and Diverse Ligand Sets – A Case Study on BACE1, TYK2, HSP90, and PERK Proteins *J.Phys. Chem. B* 2017, 121 8142-8148.

computationally intensive methodologies are incurred. We operate this proven method of molecular drug design on thousands of molecules that were chosen from a billion molecules chemical space by a fully operational quantum system.

VV: With one of your partners, Fujitsu, a major digital annealing technology provider, you are working on rapid design of lead compounds for dengue fever treatment.

Keinan: This is a project that has proven that Tachyon™ also performs efficiently with digital annealer, a quantum-inspired digital technology architecture.

There is no cure for dengue fever, a mosquito-borne tropical disease caused by dengue virus. It is said that almost half of the world's population, around 4 billion people, live in areas exposed to a risk of dengue fever. The current vaccine is effective only for people who have been previously infected, and severe Dengue is a life-threatening condition.

We have already identified potential leads. Currently they are being developed in the phase of synthesis + assays. We hope we will be able to contribute towards providing effective drug to treat this infectious disease before long.

VV: Your business strategy consists of two branches: fee for design work service and license-out of your discoveries.

Keinan: By providing molecular discovery as a service to pharma and biotech companies we get cash flow and additional wet laboratory validation. These days pharma and biotech companies are increasingly outsourcing early-stage drug discovery operations to, for instance, CROs (Chemistry Research Organization). We are pleased to help them to speed up their drug discovery process.

The other business is to license out the intellectual property of our internally developed molecules. Any inquiries are welcome.

VV Comments after the interview:

In the life science industry quantum computing is going to transform drug discovery and development along with AI. The article published this year, *"Artificial Intelligence and Quantum Computing as the Next Pharma Disruptors"*, states that "AI-QC (Quantum Computing) applications are expected to become standard in the pharma operating model over the next 5-10 years."³

³ <https://pubmed.ncbi.nlm.nih.gov/34731476/>

Tachyon™ drug design platform has already demonstrated that a paradigm shift is happening. It is interesting to observe how innovative companies like POLARIS^{qb} are going to reshape the time-consuming and costly R&D process.

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