12 Companies Using Quantum Theory To Accelerate Drug Discovery

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Molecular mechanics (MM) is a traditional computational approach when it comes to modeling in synthetic organic chemistry, medicinal chemistry, and versatile aspects of drug design. However, MM methods have significant limitations, for example, when used to study electron-based properties within the drug-receptor microenvironment. **Quantum mechanical (QM)** methods allow to substantially increase the accuracy of predictions and provide much more relevant models of chemical and biological objects and their interactions, but QM methods are extremely (often prohibitively) computationally costly.

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However, a series of advancements over recent years allowed to expand horizons in this direction, for example, the emergence of density functional theory (DFT), the overall increase in the computation power, and the emergence of distributed cloud-based computational infrastructures.

In this post, I am summarizing several notable computational companies (primarily startups), applying quantum calculations methods -- always in conjunction with other methods -- for drug discovery, and promising to boost the success rates of pharmaceutical research.

This post is a major revision and update of the original post “18 Startups Using Quantum Theory To Accelerate Drug Discovery”. Companies are listed in alphabetical order. We intend to update this post in several months -- feel free to suggest novel relevant companies to be considered for inclusion in the list.

Aqemia

Aqemia is a spin-off of École Normale Supérieure leveraging disruptive algorithms from 8 years of research led by its CEO and co-founder Dr. Maximilien Levesque. The company focuses on *de novo,* structure-based design of lead-like molecules by combining quantum and artificial intelligence (AI). A unique quantum-inspired statistical mechanics algorithm that predicts the affinity between a compound and a therapeutic target accurately and 10,000 times faster than the competition. Aqemia’s AI can generate compounds with increasing accuracy by getting feedback from the affinity predictor.

Aqemia raised a total of $11.4 million from various investors.

In February 2022, Aqemia announced a pilot study with Janssen to utilize its quantum physics-driven drug discovery technology to predict the potency of small molecules for a given target based on physics-based calculations for datasets selected by Janssen.

Hafnium Labs

Founded in 2018 in Denmark, Hafnium Labs is an early-stage research startup developing two software packages for high precision simulations of physical properties of pure components and mixtures, and for modeling electrolytes. Both software products, Q-props and Epsilon, combine the latest advances in quantum chemistry, artificial intelligence (AI), and cloud computing to achieve high accuracy of predictions.

By leveraging its cloud-based computational capabilities, Hafnium Labs accurately predicts chemistry to accelerate drug discovery, development of new materials, and processes. It also has a pay-per-use

business model, which the company claims to be more affordable, compared to usual license-based models for similar products.

So far Hafnium Labs has raised a total of $1.8 million via grant money from Innovation Fund Denmark, IBM, and Climate-KIC Acceleration Programme (EIT).

Kuano

Kuano is a UK-based company founded at the beginning of 2020. This start-up is developing novel AI and quantum solutions for designing enzymes, addressing key liabilities such as specificity, potency, and resistance.

Kuano's research platform utilizes structural data on the target enzyme or catalytic site, combining quantum simulation and quantum-inspired artificial intelligence and chemistry.

The company has In-house programs in epigenetics, protein degradation, immuno-metabolism, infectious disease, and others, while also working with partners on next-generation inhibitors of clinically and commercially validated enzyme targets.

Kuano raised a total of $1.4 million in grants and seed money from various investors, including Innovate UK and O2h Ventures.

Menten AI

Menten AI is a Canadian start-up founded in 2018, that develops a software platform for protein design powered by machine learning and quantum computing. The company uses proprietary algorithms of quantum optimization which it believes can significantly improve the accuracy of drug discovery while reducing cost and development time. The team at Menten AI created the first protein design algorithm for current and near-term quantum computers and they were the first to apply a quantum computer for designing a protein molecule.

The company claims they can perform one design cycle, from target selection to in vivo efficacy, in less than six months. Menten AI drug pipeline is currently focused on peptide therapeutics for indications with

high unmet medical needs.

Menten AI raised a total of $4 million from various investors and has partnerships with D-Wave supercomputer, IBM-Q, and a recently announced collaboration with Xanadu.

Pharmacelera

Barcelona-based computational startup Pharmacelera is applying quantum theory to boost drug design via their two primary software packages: PharmScreen and PharmQSAR.

The first tool allows for an accurate ligand-based virtual screening, using a high precision 3D ligand-alignment algorithm based on the interaction fields. It can generate a higher rate of diversity among leads, compared to classical methods and tools.

PharmQSAR is a 3D quantitative structure-activity relationship (QSAR) tool that enables a combination of multiple fields of interaction in order to perform CoMFA/CoMSIA studies.

The company was founded in 2015 and raised a total of up to $2.2 million from grants and pharmaceutical business angels.

Here is a 2020 interview with Dr. Enric Gibert, Pharmacelera's co-founder and CEO, where he answers questions about the state and future of quantum physics in modern drug design.

PharmCADD

PharmaCADD is a Southern Korea-based startup founded in 2019. The main technology platform of PharmaCADD called "Pharmulator" operates with deep neural network algorithms, molecular dynamic simulation, and quantum mechanics computation as key technologies. Pharmulator can reconstruct 3D protein structure from amino acid sequence within just several seconds.

The company collaborated with another Korean start-up Genesen to develop drugs for Multiple Sclerosis, and also signed a deal with US biotech to discover new anti-coagulant therapeutics. Recently, the company made moves to expand into India, US, and France.

The company raised a total of $22 million from SD Group and other investors.

Polaris Quantum Biotech

POLARISqb is a Durham-based developer of the world's first drug discovery software built for quantum computers, combining artificial intelligence and quantum approach. At the heart of POLARISqb technology is Tachyon*tm* drug design platform, used for executing distributed molecular design work across the cloud, managed by an automated process that allows for searching large chemical libraries, while running multiple projects in parallel. By developing proprietary software for quantum systems, the company claims it can substantially accelerate drug design and get leads of higher quality. Due to the inherent “agnosticism” of *Tachyontm* system, it is able to work in multiple diseases and indications.

In 2020, POLARISqb partnered with Fujitsu to jointly develop a research platform to speed up the discovery of treatments for Dengue fever and other indications. In 2021, POLARISqb entered a collaboration with Auransa to focus on neglected women's diseases. In 2022, POLARISqb entered a collaboration with PhoreMost to bring the power of quantum computing to search for new cancer therapies.

The company raised a total of $2.1 million to develop its platform.

ProteinQure

Founded in 2017, Toronto-based startup ProteinQure is combining quantum computing, reinforcement learning, and atomistic simulations to design novel protein drugs. Using this mix of technologies they model essential processes, such as protein folding, and the underlying physics of interactions between biomolecules.

Using their proprietary algorithms and external supercomputing resources, ProteinQure can design small peptide-based therapeutics (including cyclic peptides), and explore protein structures without known crystal structures.

The company raised a total of $4.6 million from various investors, including Creative Destruction Lab and Felicis Ventures.

Riverlane

The website of UK-based Riverlane reads “the world's first quantum engineering company.”. Founded in 2016 in Cambridge, the company raised a total of $24.1 million to advance its quantum hardware and software technologies for a wide range of applications, including pharmaceutical research and chemistry.

In July 2021, Riverlane joined forces with Rigetti Computing, alongside existing partners Astex Pharmaceuticals, to advance quantum computing for drug discovery.

A notable project by Riverlane is their operating system for quantum computers – Deltaflow.OS®, which addresses one of the bottlenecks of quantum computing today: quantum error correction.

Roivant Discovery

Roivant Discovery is the scientific subsidiary of Roivant Sciences (NASDAQ: ROIV), a publicly-traded umbrella company, founded in 2014 by Vivek Ramaswamy. Roivant Discovery was formed by acquiring Boston-based computational drug discovery company Silicon Therapeutics -- a developer of a research platform combining physics-based molecular simulations, quantum physics, statistical thermodynamics, and molecular dynamics for the improvement of conventional drug discovery.

Silicon Therapeutics was focused on innate immunity in cancer and inflammation, and it had developed its own discovery pipeline of early small molecule drug candidates (4 in a discovery phase and 2 in the pre-clinical phase, as of June 2019). The company was also active in the field of conformational genetics, linking genetic mutations with biological functions.

In February 2021, Roivant Sciences acquired Silicon Therapeutics for $450 million in Roivant equity, with additional potential regulatory and commercial milestone payments.

XtalPi

Founded in 2014 by a group of quantum physicists at MIT, XtalPi is a quantum physics-based, AI-powered drug R&D company with the mission to revolutionize drug discovery and development by improving the speed, scale, novelty, and success rate. While headquartered in Boston, the company also has a major operational and research presence in China.

Its Intelligent Digital Drug Discovery and Development (ID4) platform, incorporating quantum mechanics, artificial intelligence, and high-performance cloud computing algorithms, allows predicting with high precision physiochemical and pharmaceutical properties of small-molecule drug candidates, as well as their crystal structures -- critical elements in successful drug R&D.

By this time, XtalPi raised a staggering amount of $786.4 million from numerous investors, including Sequoia China, Tencent, and Google, which makes it one of the most well-funded computational drug discovery startups on the market. The company has multiple research collaborations with pharmaceutical companies, including Pfizer.

Zapata Computing

Boston-based Zapata Computing is a quantum software company that offers computing solutions for industrial and commercial use for a number of use cases, including pharmaceutical research. Zapata was founded in 2017 and originated in the laboratory of Alán Aspuru-Guzik at Harvard, where he had been developing quantum computing methods for chemical simulations.

Zapata raised a total of $67.4 million from multiple investors, including Prelude Ventures, and Comcast Ventures. The company has built its research platform “Orquestra”, which combines a powerful software platform and quantum algorithm libraries for applications in chemistry, biopharma, machine learning, and optimization.

Read or listen to our interview with Dr. Christopher Savoie, Co-founder, and CEO at Zapata Computing, where he explains the current state of quantum computing, existing opportunities, and challenges, and provides his vision about what is coming next in the exciting field of quantum computing and quantum theory applications in drug discovery.

- ApexQubit

- Aqemia
- ChemAlive SA
- FAR Biotech
- Hafnium Labs
- Kuano
- Menten AI
- PharmCADD
- Polaris Quantum Biotech
- ProteinQure
- Riverlane
- Silicon Therapeutics
- XtalPi
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