Simulation & Optimization for BioPharma

New drugs take anywhere from 10-15 years and $1.3B-$4B to create—far too slow and expensive for patients and payers.

Our AQ technology combines the versatility and speed of AI with the accuracy of quantum simulation to make drug development cheaper and faster, while reducing risk in clinical trials. Our quantum simulations predict the electronic interactions between molecules at better-than-lab accuracies. AI accelerates these simulations, connects them to real-world drug discovery workflows, and adds qualitatively new capabilities such as de novo drug discovery.

We pair these technologies with an experienced computational drug discovery team, working hand-in-hand with partners to customize AQ to their specialized needs, and to pave the way for groundbreaking new medicines. At SandboxAQ, we are not satisfied with improvements to the status quo. We strive for an unrecognizably advanced future.

Simulations & Optimizations

SandboxAQ's simulations provide greater accuracy of binding affinities to account for quantum interaction effects and thus improve lead optimization using simulated variants.

With simulations, we can computationally test new small molecule drugs or peptides, including for first-in-class or rare-target programs. We can optimize these tests over chemical space automatically. By bringing these processes in silico, we dramatically reduce the downstream risks of drug discovery.

Fewer candidates need to be selected for further benchtop chemistry pre-clinical evaluations, leading to a cheaper and faster process to test candidates before clinical trials.

This leads to higher target effectiveness of trialed candidates, thus lowering the clinical trial failure risk.

$1-4
Billion

10-15
Years

60+%
Failure

Drug Discovery Today

The AQ Technology Difference

AI tools allow computers to learn complex new tasks such as de novo drug discovery, but the results can be inaccurate. Quantum simulations can reach very high accuracies, but the process to get there is expensive and specialized. Our AQ tools make no sacrifices: they can be utilized with today's classical hardware to radically shift the economics of drug discovery.

We use AI, HPC/GPU, and tensor networks (a method to simulate quantum systems with classical hardware) to achieve tangible drug discovery impacts.

AQ Accelerates Drug Discovery

- ☑ **Protein-ligand binding prediction**
- ☑ **RNA folding**
- ☑ **Free energy of binding**
- ☑ **Protein structure simulation**
- ☑ **AI- and quantum- enhanced virtual screening / lead optimization**
- ☑ **Combination therapy**

Learn More

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