SANDBOXAQ

AI + Quantum (AQ) Simulations for Drug Discovery

AQ simulations allow us to perform quantum simulations with classical advanced hardware before fault tolerant quantum computers arrive

How We Work

- ✓ We deliver end-to-end, custom computational solutions
- ✓ Accessible to standard hardware via machine-learned overlays
- ✓ Physical simulation and optimization
- ✓ With cutting-edge advanced computations via HPC/GPU and tensor networks (a computational method enabling classical computers to simulate weakly entangled quantum systems)

Example Problems We Could Tackle Together

- Protein-ligand binding prediction
- Crystal structure simulation
- AI- and quantum-enhanced virtual screening / lead optimization

Email us at info@sandboxaq.com to learn more.

Customer Journey Map

PROBLEM

1

Neurodegenerative diseases are extremely challenging for drug discovery with a large number of clinical failures in recent years, including expensive Phase 3 clinical trials. This medical need has limited effective treatments on the horizon.

2

A world-renowned drug discovery laboratory linked specific high-order biopolymer conformations in the brain to several neurodegenerative diseases. An opportunity arose to accelerate the drug discovery progress via improved understanding of the relationship between molecular properties and disease progression.

3

In particular, a lack of structural understanding of ligand-target interactions at a molecular level slowed traditional medicinal chemistry optimization, driven mainly by phenotypic screening.

SOLUTION

4

Recently, the group successfully resolved CryoEM structures of the ligand-target complex, revealing new and unexpected binding modes: There was an exceptional opportunity to understand the ligand activity at a molecular level.

5

No commercially available solutions were able to reproduce the unconventional observed ligand-target binding mode. SandboxAQ worked in close collaboration with the group, taking advantage of their unique expertise and insights to design an optimal bespoke computational method to meet this need.

IMPACT

6

The project team translates the novel structural information into a testable hypothesis to understand the small molecule mode-of-action. For the first time in 30 years, rational structure-based drug discovery against these targets becomes possible.

7

This novel solution is able to predict binding positions & affinity between investigational new drugs & the misfolded protein, combining molecular docking, quantum simulation, AI, molecular dynamics and absolute free energy perturbation (FEP).

8

The platform has the potential to enable unprecedented virtual screening strategies against large compound libraries, potentially increasing the hit rate by 10x compared to traditional HTS, leading to time and cost improvements though the entire drug discovery pipeline, and saving 1-3 years of research, $25-75M, and 270K lives/year.