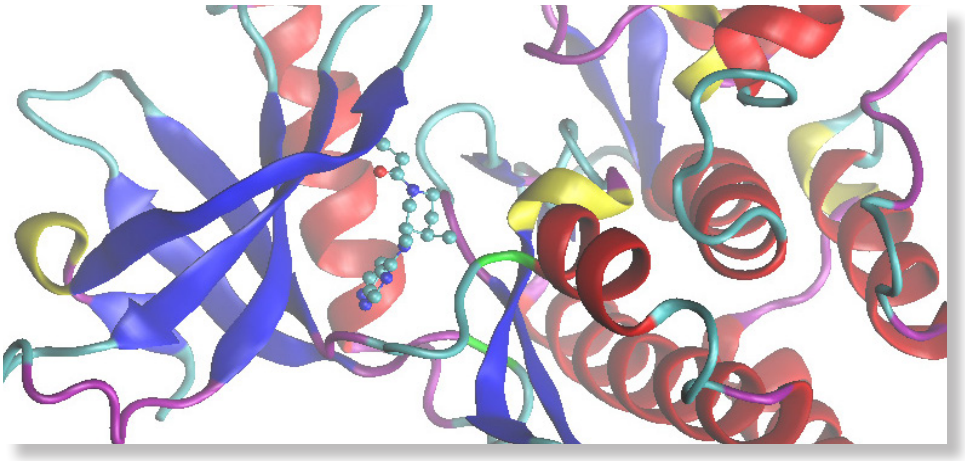
CloudPharmaceuticals

Speed the Discovery of Novel Drug Candidates with Quantum Molecular Design

Cloud Pharmaceuticals' Quantum Molecular Design℠ process represents a paradigm shift that dramatically improves upon traditional drug discovery and design methods. This proprietary process combined with cloud computing and strong relationships with partners across industry and academia forms a single platform that enables the rapid and accurate discovery, design, and development of new therapeutics to improve human health and well-being.

Key Capabilities:

- Use of highly accurate computational algorithms to accurately predict binding affinity of small molecules
- Generation of novel composition of matter leading with complete freedom to operate
- Seamless discovery, design, and early development from a single platform



Quantum Molecular Design discovers novel drug candidates by searching the virtual space of millions of molecules, accurately calculating binding affinities between targets and selected candidates, and filtering them for toxicity and drug-like properties.

Search Vast Virtual Libraries

It is generally recognized that drug discovery and development are very time- and resource-consuming processes. Designing new drugs that bind to a specified protein target requires finding the best molecule in a vast chemical space. With an estimated 10^{65} stable molecules with a molecular weight below 850 available for exploration, researching this space by direct enumeration and evaluation is prohibitively costly.

Quantum Molecular Design enables a more efficient search of chemical space. This process uses reverse engineering methods to solve the problem of going from a set of desired properties back to realistic chemical structures and material morphologies that may have these properties.

Calculate Binding Affinities with Greater Speed and Accuracy

Accurately calculating binding affinities between a protein and a small molecule is critical to rationally designing new drugs. The Quantum Molecular Design process runs computational models to quickly generate and scan virtual chemical libraries to find the strongest inhibitors of a specific biological target. The process identifies novel drug candidates that feature good clinical trial properties and demonstrate low probability of toxic side effects. This process is ideal for universities seeking to identify leads for novel targets as well as biotechnology and pharmaceutical companies that are developing new drugs.

Explore the Quantum Molecular Design Process

The Quantum Molecular Design process begins with a 3-D model of the target, which is entered into the computer model (see figure). A training set is used, if available, to calibrate the run. If no training set is available, a two-step run and a binding assay are used to set up the run.

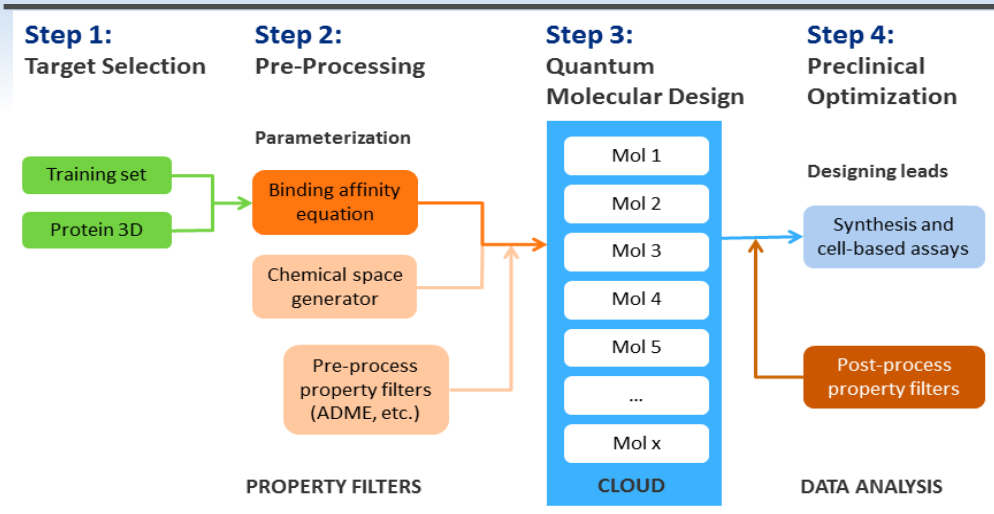


FIGURE: Quantum Molecular Design Process

Quantum Molecular Design uses the full Schrödinger wave equation and an accurate solvation model to calculate binding affinity. A targeted set of "hot spots" in chemical space are generated automatically. Property filters are used to ensure that chosen candidates are of low toxicity, possess good drug-like properties, and are able to be synthesized. Then Quantum Molecular Design employs an artificial-intelligence search through this space to discover candidate drugs. The computing power available on the cloud ensures this result can be obtained quickly.

Enable Rapid and Accurate Drug Discovery

Use of Quantum Molecular Design for discovery of novel drug candidates is very fast when compared to brute force free-energy calculations, especially those done with quantum mechanics (see table). Further, it produces accurate results when compared to traditional docking algorithms that only approximate binding. That's because Quantum Molecular Design can target and search novel molecular space more efficiently.

	Quantum Molecular Design	Docking	Free-Energy Calculation
Speed	Very Fast	Very Fast	Very Slow
Accuracy	High	Low	High
Novelty	High	Low	Low

The binding affinity accuracy of Quantum Molecular Design is 70-90%, compared with 20-30% for traditional docking algorithms. The significance of this improvement is magnified by using Quantum Molecular Design to discover targets that are selective against specified proteins (i.e. the molecule will only bind to the target protein), which is a critical feature to minimize toxic effects.

Partner with Cloud Pharmaceuticals

Cloud Pharmaceuticals partners extensively throughout the development process. We use our proprietary methods, along with a network of virtual partners, to fill the need that industry and academia have for rapid development of new active molecules. We seek partners at all stages of drug development, including early stage, preclinical, IND, and Phase 1 and 2.

Visit www.cloudpharmaceuticals.com or send an e-mail to info@cloudpharmaceuticals.com to learn more about Quantum Molecular Design and partnering with us.

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