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AI and Quantum Research Center (AIQRC), Asia University, Taiwan

Activities

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Quantum-Inspired Innovations in De-Novo Drug Discovery

Drug discovery is a complex and high-risk process. Developing new molecules that effectively target disease-related proteins while ensuring safety and efficacy often takes years and comes with high costs. Many promising candidates fail before reaching approval, highlighting the urgent need for faster, more efficient approaches to identify potential therapeutics. One of the biggest challenges is exploring enormous chemical spaces containing billions of molecules—a scale that traditional computational methods struggle to handle.

To overcome this limitation, researchers are turning to quantum-inspired technologies, such as Fujitsu's Digital Annealer (DA). Unlike conventional computers, the DA leverages optimization techniques inspired by quantum mechanics, including phenomena like quantum tunneling, to navigate complex molecular landscapes efficiently. While not a true quantum computer, the DA's fully connected digital architecture can solve large-scale combinatorial optimization problems with remarkable speed and accuracy, making it ideal for early-stage drug discovery.

In a recent study, the Digital Annealer (DA) was applied to a chemical library of approximately 1.3 billion molecules to identify around 1,000 optimal candidates for further high-accuracy evaluation. The optimization process was guided by two sets of constraints. The first set focused on general drug-like characteristics that apply broadly to drug discovery efforts. These included parameters such as molecular weight (450–500), hydrogen bond donors (2–5), hydrogen bond acceptors (2–10), topological polar surface area (90–140), rotatable bond count (4–8), and lipophilicity, expressed as the octanol–water partition coefficient (LogP, 0–5). Additional functional group filters, as described in the GDB-17 database, were applied to exclude unrealistic or potentially toxic structures, and synthetic accessibility was evaluated for each candidate. The second category focused on structural constraints specific to the Dengue Fever RdRp allosteric pocket. These constraints defined critical distances between key pharmacophoric features based on the bound conformation of compound-23 in the 5HMZ.pdb structure. Specifically, the distances between one hydrogen bond donor and two hydrogen bond acceptors (corresponding to –OH, –C=O, and –S=O groups, respectively) were constrained to

ensure effective binding. Only molecules satisfying all drug-like and target-specific constraints were considered optimal and selected from the full chemical library.

The DA used a Quadratic Unconstrained Binary Optimization (QUBO) algorithm to search, running approximately 40 iterations across the library. Each run took just 0.6 seconds to select 125 candidate molecules, from which the top 25 were retained—resulting in 977 high-quality molecules. This approach represents a significant advance in de novo drug design. By scanning billions of molecules in seconds, the Digital Annealer generates thousands of synthetically feasible lead candidates in minutes. This not only accelerates early-stage drug discovery but also increases the chances of identifying innovative molecules with therapeutic potential. Quantum-inspired technologies, such as the Digital Annealer, are poised to become indispensable tools for faster, smarter, and more efficient drug development in the fight against complex diseases.

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