SandboxAQ: Your Partner For Drug Discovery's Toughest Challenges

Creating specialized solutions with Large Quantitative Models

You have an undruggable target. We have the AI + physics-based solutions to solve it.

AQBioSim reaches beyond the capabilities of chemical generative AI models that struggle to make accurate predictions outside their training dataset. We can expand the chemical space with provably accurate predictions by combining physics-based modeling with advanced AI methodologies.

More hits and diverse molecules at a lower cost—and years of research time saved.

Small Molecule Discovery

Using our physics-based AI approach, you can **screen thousands of ligands efficiently and expand your search to billions of compounds**. AQBioSim allows for virtual screening of a wider variety of targets than traditional methods—**facilitating better drug discovery against undruggable targets** like those found in neurodegenerative diseases. We utilize an active-learning-enhanced absolute free energy perturbation workflow with a novel generative chemistry AI incorporating deep diffusion and multi-objective optimization for structure-based drug design. Our platform integrates this technology and knowledge graphs to efficiently identify small molecules with optimal binding affinity, **maximizing successful search outcomes and minimizing risk**.

Antibody and Biologics Optimization

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mRNA Therapeutics

We leverage Bayesian optimization and coarse-grained simulations to **fine-tune mRNA designs for peak performance**. Our physics-based molecular dynamics modeling optimizes lipid nanoparticle (LNP) delivery, enhancing formulation stability and therapeutic efficacy. Knowledge graph-driven neo-epitope selection ensures precise targeting, **unlocking the full potential of mRNA therapies** and improving their therapeutic outcomes.

Clinical Development & Biomarker Discovery

AQBioSim enables seamless and secure data integration powered by graph foundation models and advanced probabilistic querying capabilities. Our advanced knowledge graphs integrate comprehensive open-source data, biomedical ontologies, raw RNAseq and NGS data, and the latest literature. **Users can intuitively explore and interrogate complex knowledge graphs and model-derived outputs** with our interactive querying interface. This approach brings accessible, biologically interpretable, and actionable insights for biomarker identification, drug mechanism of action, patient stratification, and more.

Let's Collaborate

AQBioSim drives innovation across therapeutic areas, including immunology, oncology, neurology, and rare diseases. We actively collaborate with leading pharma, biotech, and academic institutions across 15+ pipelines.

Stop tackling your drug discovery challenges alone. Contact us at simulations@sandboxaq.com to explore how AQBioSim can create tailored solutions for your specific needs today.

Learn More www.sandboxaq.com/biosim