How sequence-based AI achieve whole genome screening for billions of small molecule and antibody candidates in hours

Destructed Drug Discovery: Sequence-Based AI for Rapid Evaluation of Small Molecules and Antibodies”

SAN FRANCISCO , CA, UNITED STATES, January 14, 2026 /EINPresswire.com/ -- Ainnocence today announced a major milestone in artificial-intelligence driven drug discovery in the white paper by C&EN: a sequence-first AI platform capable of screening billions of small-molecule and antibody candidates across the entire genome in hours on a single GPU without relying on 3D structural modeling.

> Drug discovery is a multi-parameter optimization problem, miss one constraint and the candidate fails,”
>
> *Dr. Lurong Pan, CEO of Ainnocence*

This approach represents a fundamental shift in how therapeutic candidates are discovered, replacing decades of structure-dependent simulations and computationally expensive systems such as AlphaFold with direct learning from biological sequences and experimental data. The result is a scalable, faster, and 10 thousand times more cost-efficient paradigm for early-stage drug discovery.

From Structure Bottlenecks to Sequence Intelligence

Traditional AI drug discovery pipelines are constrained by protein structure availability and limited 3D structure prediction in meso, computationally intensive molecular dynamics, and limited throughput. By contrast, Ainnocence’s platform operates entirely at the sequence level, enabling:

- Whole-proteome virtual screening without solved structures
- Billions of candidates evaluated in hours, not months
- 80% reduction in wet-lab cost and time
- 10–60% experimental hit rates, far exceeding industry averages
- 60+ successful screening projects
- Cover all target families and naturally disordered proteins and motif

“Drug discovery is a multi-parameter optimization problem, miss one constraint and the

candidate fails," said Lurong Pan, Founder and CEO of Ainnocence. "Sequence-based AI allows us to optimize binding, specificity, developability, and manufacturability simultaneously, at a scale to whole genome level that was previously impossible."

Validated at Global Scale and in a Pandemic

The platform has been applied across 60+ therapeutic programs, including antibodies, small molecules, cell therapies, siRNA, and synthetic biology applications. In one landmark study, Ainnocence computationally designed mutation-resistant antibodies against SARS-CoV-2 variants, successfully predicting neutralizers for Delta and Omicron before Omicron emerged, demonstrating the model's ability to learn evolutionary patterns directly from sequence data.


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DESTRUCTURED DRUG DISCOVERY: HOW SEQUENCE-BASED AI SPEEDS AND EXPANDS THE SEARCH FOR NEW THERAPEUTICS

Scientists must venture through a vast chemical space to identify potential drugs: it's estimated that 10^{60} different small molecules obey the standard rules of bioavailability, a tally greater than the number of seconds that have elapsed since the Big Bang. Biologics, an important class of modern drugs that includes antibody therapeutics, expand this space further.[1,2] Identifying a promising drug candidate from this immense pool of possibilities requires years of research and millions of dollars of investment. Even then, the likelihood that a drug moves from Phase I trials to market approval ranges from only 8–12%.[3,4]

"Drug discovery is always a multiparameter optimization problem," says Lurong Pan, founder and CEO of Ainnocence. "If even one parameter is missing, the whole drug candidate will fail." To shorten drug development timelines, reduce costs, and get more treatments to patients, scientists require tools that help them balance this optimization problem and make sense of massive chemical spaces. Many within the field of drug discovery are betting on artificial intelligence models to be that tool.

That bet is beginning to pay off. More companies are relying on AI's predictive powers to inform drug discovery, and promising examples are emerging. For example, the small molecule rentosertib may soon become the first drug designed by generative AI methods to enter Phase 3 trials. It likely will not be the last.[5,6]

AI gives drug developers a new way to search for theoretical therapeutics. However, AI advances to date have largely focused on predicting the 3D structure of human protein targets and how drug molecules interact with them.[7–9] According to Pan, these structural simulations rely on expensive and imperfect data to train computationally expensive algorithms.

Pan believes the solution to this problem is to bypass structural modeling altogether and instead use proteins' amino acid sequences to guide AI models.

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Featured in C&EN: Discover how sequence-based AI is transforming drug discovery, accelerating and broadening the search for new therapeutics

Internal benchmarks show that Ainnocence's protein foundation models achieve Spearman correlation performance comparable to structure-based models, while requiring orders of magnitude less compute and running efficiently on a single GPU.

Recognized by C&EN and the American Chemical Society

This breakthrough has been featured in the white paper Chemical & Engineering News (C&EN) the flagship news outlet of the American Chemical Society, underscoring the scientific and industrial significance of Ainnocence's approach.

C&EN highlighted how sequence-based AI bypasses the limitations of structural snapshots, leverages vastly more abundant experimental data, and unlocks scalable discovery across chemical and biological space marking a turning point similar to the inflection moments seen in large language models and protein foundation models.

A Platform, Not a Point Solution

Ainnocence's technology stack includes:

- SentinusAI® for antibody and protein therapeutics
- CarbonAI™ for small-molecule, PROTAC and pocket discovery from sequence alone
- CellulaAI™ for multi-epitope cell therapy design

- NatmolAI™ & BioSynthAI™ for natural products and synthetic biology

Each platform continuously retrains on experimental feedback, compounding intelligence with every program.

What Comes Next

As biological data volume continues to grow, sequence-based AI is poised to become the dominant discovery layer across pharma, biotech, and industrial biology. Ainnocence is expanding partnerships, integrating human-relevant microphysiological systems, and extending its models toward late-stage optimization and translational prediction.

“Humans can’t intuitively see chemistry from letters,” Pan said. “But AI can. And once it does, the entire drug discovery landscape changes.”

Collaborate with Ainnocence

Ainnocence is open to collaboration with academic groups, biotechnology companies, and industry partners interested in applying Ainnocence platforms, supporting joint development projects, pilot studies, and long-term partnerships tailored to specific needs.
For collaboration inquiries, contact service@ainnocence.com or visit www.ainnocence.com.

About Ainnocence

Founded in 2021 and headquartered in California, Ainnocence is a next-generation biotechnology company transforming drug discovery and synthetic biology through AI-based, sequence-first engineering. The company’s self-evolving platform evaluates up to 10 billion molecules spanning proteins, antibodies, small molecules, nucleic acids, and chemical formulations within hours to weeks, enabling rapid, multi-objective design across therapeutic, biological, and chemical systems. By reducing R&D timelines and costs while increasing success rates, Ainnocence empowers industry and academic partners to pursue complex biological innovation with greater precision and control.

Lurong Pan, PhD
Ainnocence
+1 205-249-7424
service@ainnocence.com
Visit us on social media:
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