

Ainnocence's CarbonAI®, a Proprietary AI Engine for De Novo Small-Molecule and PROTAC Design and Optimization

Platform screens up to 10 billion compounds in hours, delivering wet-lab-ready candidates in weeks without requiring 3D protein structures

SAN FRANCISCO , CA, UNITED STATES, March 30, 2026 /EINPresswire.com/ -- Ainnocence, a next-

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Dr. Lurong Pan, Founder and CEO of Ainnocence

generation AI drug discovery company, announces the commercial availability of CarbonAI®, its proprietary artificial intelligence engine for de novo small-molecule and PROTAC design. CarbonAI® enables pharmaceutical and biotechnology organizations to advance from target sequence to optimized, wet-lab-ready lead candidates in weeks compressing a process that traditionally spans years.

“The fundamental bottleneck in small-molecule discovery has not been a lack of chemical matter, it has been the inability to explore vast chemical spaces while simultaneously optimizing for the properties that

determine clinical success,” said Dr. Lurong Pan, PhD, Founder and CEO of Ainnocence.

“CarbonAI® was designed from the ground to solve that problem. By working directly from sequence, we enable programs that were previously intractable due to missing or unreliable structural data. We are compressing discovery timelines from years to weeks and giving our partners the confidence to advance candidates with strong multi-parameter profiles from day one.”

CarbonAI® operates entirely from amino acid sequence input, eliminating the dependency on experimental 3D protein structures that constrains conventional and many AI-driven approaches. The platform screens chemical space at a scale of up to 10 billion compounds within hours to days, simultaneously optimizing across potency, selectivity, ADME/Tox, synthetic accessibility, and IP novelty. Uniquely, CarbonAI® is a pioneer small-molecule engine capable of whole-genome off-target screening in hours enabling safety profiling at a scale that is simply not achievable with conventional docking or structure-based methods. Key platform benchmarks

include:

- Virtual screening AUC of 0.981 (DUD.E) and 0.974 (DUD), with mean Enrichment Factor EF@2% of 39.7 (DUD.E) and 36.2 (DUD) state-of-the-art on established benchmarks running 16,000× faster than conventional docking software; ~360,000 compounds screened per CPU-hour, fully scalable with parallel processing
- Protein-ligand binding prediction AuROC of 0.988 (structure-based) and 0.939 (sequence-based), vs. 0.8 average for conventional docking tools
- Proprietary training dataset: 267,872 ADME/Tox data points supporting 35 AI models; 564,046 target binding entries with 1,379 proteins; covering 2B virtual and real chemical spaces
- 30+ ADME/Tox pharmacological properties predicted simultaneously, including CYP inhibition (AuROC 0.90), hERG inhibition (0.88), blood-brain barrier permeability (0.95), and clearance (0.95)
- Training sets up to 25,000 data points per ADME endpoint, substantially exceeding competing academic and commercial packages
- 10%-60% hit rate on wet-lab validation across 60+ completed programs
- Pioneer small-molecule AI engine capable of whole-genome off-target screening in hours-identifying compound toxicity and selectivity risks across the full proteome simultaneously, an efficiency unavailable in any competing platform

AI-driven drug discovery has emerged as a central strategic priority for pharma and biotech organizations seeking to compress timelines, reduce costs, and improve the quality of candidates entering preclinical development. CarbonAI® has delivered proven results across partner programs:

- 60+ therapeutic programs completed with wet-lab validation and demonstrated milestone success
- 50 ranked candidates delivered across 3 iterative optimization cycles, advancing to wet-lab testing within approximately 2 weeks of project kick-off
- Hits-to-lead in under 2 months vs. the traditional 2-year standard, with up to 80% cost reduction vs. HTS approaches requiring 10 million- one billion screening compounds
- Generative model optimizes 30 pharmacological properties simultaneously with 400K+ chemical space coverage

Explore the Platform

Discover how CarbonAI® supports AI-driven discovery by transforming complex biological data

into actionable insights. Our platform overview demonstrates how CarbonAI® helps research teams analyze targets, prioritize candidates, and streamline decision-making across the discovery pipeline. [Watch the Platform Overview](#)

Get Access to CarbonAI®

CarbonAI® is now available for organizations interested in integrating AI into their therapeutic discovery workflows. Flexible engagement options allow teams to adopt the platform in ways that best support their research goals and development timelines. [Explore Access Options and Pricing](#)

Connect With Our Team

If you would like to learn more before getting started, schedule a conversation with the Ainnocence team. During this session, we can discuss your research objectives, demonstrate relevant platform capabilities, and explore how CarbonAI® could fit into your existing discovery programs. [Request a Discovery Meeting](#)

About Ainnocence

Ainnocence is a next-generation AI drug discovery company founded in 2021 and headquartered in Mountain View, California. The company's platform encompasses generative AI platform to screen up to 10 billion molecules within hours to accelerate drug discovery, CarbonAI® for small-molecule and PROTAC design, SentinusAI® for antibody engineering, CellulaAITM for cell therapy, NatmolAITM for natural product discovery, and additional AI engines spanning target assessment and biosynthesis. Ainnocence partners with pharmaceutical and biotechnology organizations to compress discovery timelines and improve the quality of candidates advancing into development. For more information, visit ainnocence.com.

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