Redefining Chemistry: How AI Shrinks Small-Molecule Discovery from Years to Weeks

SAN FRANCISCO, CA, UNITED STATES, September 25, 2025 /EINPresswire.com/ -- Ainnocence today unveiled a major advance in AI-driven small-molecule R&D, demonstrating how its platform compresses the upfront discovery cycle from years to mere weeks, without compromising rigor on potency, selectivity, and developability.

> Chemistry shouldn't take years to show you what's possible"
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> *Dr. Lurong Pan, CEO of Ainnocence*

Built on Ainnocence's third-generation AI system and its CarbonAI® design engine, the platform unifies generative chemistry, physics-aware scoring, ADME/Tox prediction, and rapid iteration into a closed-loop workflow. In internal and partner programs, this has translated into swift progression from target hypothesis to synthesized, test-ready lead series in a fraction of traditional timelines.

"Chemistry shouldn't take years to show you what's possible," said Dr. Lurong Pan, CEO of Ainnocence. "By combining large-scale generative models with multi-objective optimization and instant manufacturability checks, we turn weeks into the new unit of progress for small-molecule discovery."

What's new

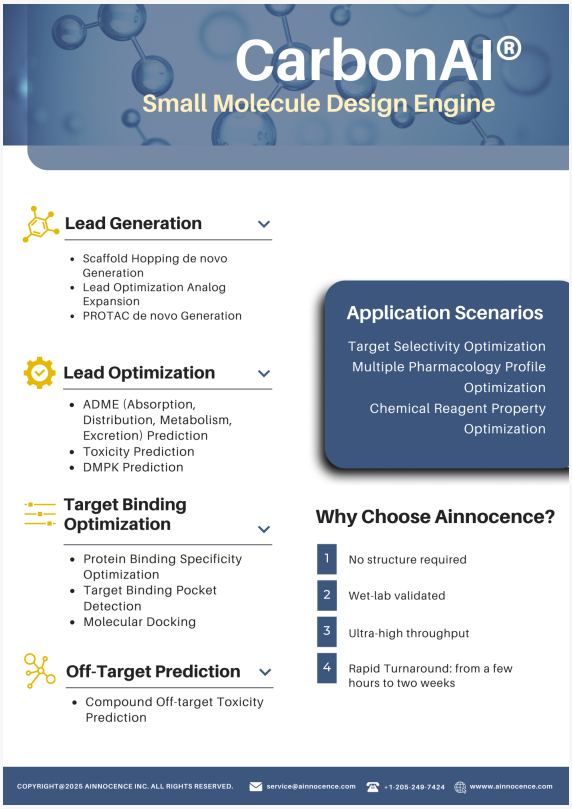
• Weeks, not years: Rapid progression from initial design brief to prioritized lead series via continuous AI-guided cycles.
• Massive search at practical cost: Virtual screening and design exploration across libraries up to 10^10 compounds within hours, focusing compute where it matters most.
• True multi-objective design: Simultaneous optimization for potency, selectivity, ADME/Tox, IP-friendly novelty, synthetic accessibility, and cost-of-goods, all scored in one loop.
• CarbonAI® for small molecules & PROTACs: CarbonAI® is a de novo small-molecule and PROTAC AI design engine capable of screening billions of compounds in mere days, simultaneously optimizing multiple pharmacological properties for lead generation and optimization. It delivers 50 candidates in 3 iterations for wet-lab testing, with milestone success achieved.

How it works

1. Design brief in: Define target, desired MoA, liabilities to avoid, and developability constraints, all captured in a structed digital template.
2. Generate & score: Physics-informed generative models propose candidates; property predictors and AI/ML scorecards rank them.
3. Select & synthesize: Shortlisted compounds move directly into synthesis with vendor-ready routes and procurement lists.
4. Close the loop: Wet-lab results feed back to the models for rapid, data-driven improvement ensuring each cycle is faster and smarter than the last.

Early access & partnering

Ainnocence is opening CarbonAI® Accelerator slots for biopharma, specialty chemicals, and advanced materials teams seeking to compress timelines or rescue stalled programs. Partners gain hands-on access to the platform, optional on-prem deployment, and dedicated AI-chemistry support.



Ainnocence's CarbonAI® Platform for AI-Powered Small Molecule Drug Design — Enabling De Novo Generation, Lead Optimization, and Off-Target Prediction Without Structural Data

About Ainnocence

Ainnocence is a next-generation biotech and deep-tech company building AI for molecular discovery across therapeutics, synthetic biology, and advanced materials. Its third-generation AI platform delivers lightning-fast virtual screening and multi-objective profile optimization, with computational capacity reaching billions of sequences or compounds within hours, enabling high wet-lab hit rates and dramatically reduced discovery time and cost. Learn more at www.ainnocence.com.

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