NatmolAI™: Computational Expansion and Optimization of Natural-Product Chemical Space

SAN FRANCISCO , CA, UNITED STATES, January 9, 2026 /EINPresswire.com/ -- Ainnocence, a next-generation AI-driven biotechnology company, announces NatmolAI™, a sequence-first molecular design platform focused on the discovery and engineering of natural-product-inspired small molecules and bioactive compounds. Drawing on an 800k+ curated natural-product library with source origin tracking, NatmolAI™ enables systematic exploration, optimization, and redesign of complex natural chemical space using biologics-grade computational precision, delivering high-confidence hit lists in hours and experimentally validated leads within a month, with milestone success typically requiring wet-lab testing of just a few dozen compounds across 2–3 iterations.

> Our goal with NatmolAI™ is not to replace natural products, but to understand and extend them”
>
> *Dr. Lurong Pan, CEO of Ainnocence*

Natural molecules remain a foundational source of bioactive compounds, yet their discovery and optimization are constrained by scarcity, structural complexity, and limited tunability. NatmolAI™ addresses these limitations by decoupling molecular design from physical isolation, allowing nature-derived chemical principles to be explored, expanded, and optimized computationally before experimental validation. This approach tackles key challenges like limited scalability, ADME deficiencies, and sourcing complexities through integrated multi-objective optimization, SAR analysis, and biosynthetic context annotations, empowering sustainable, green drug discovery with lower toxicity profiles and superior tolerability compared to synthetic alternatives.

From Natural Product Discovery to Computational Molecular Design

Traditional natural product research depends on extraction, fractionation, and bioactivity-guided screening, processes that are slow, low-throughput, and limited to what can be physically isolated from biological sources. Subsequent chemical optimization typically relies on iterative synthetic modification with limited systematic guidance.

NatmolAI™ shifts natural product discovery from isolation-driven workflows to design-by-sequence. Starting from known natural scaffolds, biosynthetic motifs, or target-defined

functional requirements, the platform generates large populations of candidate molecules in silico, evaluating up to 10 billion chemical spaces over hours. Candidates are prioritized using learned relationships between molecular patterns, physicochemical properties, and biological activity, enabling systematic exploration of chemical space beyond naturally occurring compounds while preserving desirable bioactive characteristics.

NatmolAI™, Natural Molecule AI Engine

Learning and Expanding Nature's Chemical Space

NatmolAI™ learns how stability, solubility, selectivity, and manufacturability correlate with molecular sequence patterns and composition, and uses those learned relationships to guide redesign.

"Our goal with NatmolAI™ is not to replace natural products, but to understand and extend them," said Lurong Pan, PhD, Founder and CEO of Ainnocence. "NatmolAI™ uses generative AI modeling to systematically expand natural product chemical space and prioritize variants with improved developability."

Multi-Objective Optimization Beyond Single-Property Design

NatmolAI™ is built to optimize across multiple objectives simultaneously, reflecting the real constraints of downstream development. Candidate molecules are evaluated computationally for predicted target relevance and interaction likelihood, physicochemical balance, stability, and early risk signals relevant to safety and formulation.

Rather than optimizing potency in isolation, the platform resolves trade-offs at the design stage, producing candidates that are balanced across performance and developability criteria. This multi-objective optimization computational front-loading reduces the need for broad experimental screening and screening and focuses laboratory validation on a narrow set of high-probability molecules.

NatmolAI™ – Natural Molecule Discovery Engine

Natural Molecule Virtual Screening: Screens an 800K+ curated natural-product database to identify target-based binders, with source origin tracking, availability, Structure-Activity Relationship (SAR) analysis, and Natural Product Similarity Search. Ideal when starting without

leads or exploring new nature-derived chemical spaces.
Pharmacological Optimization: Enhances ADME, bioavailability, and metabolic stability through scaffold modifications and biosynthetic pathway analysis while preserving natural character. Perfect for improving developability of natural hits.
Drug Repurposing: Mines traditional medicine data for multi-target activity predictions, cross-indication potential, and synergistic combinations. Use to uncover new uses for existing natural assets in therapeutics or nutraceuticals.
Target Analysis & Selectivity Profiling: Predicts target association likelihood, prioritizes selectivity trends across targets, and supports mechanism inference through sequence-activity correlations and comparative analysis. Used throughout for efficacy guidance and early safety de-risking.
NatmolAI™ supports areas including nutraceutical development, traditional medicine modernization, green drug discovery, and botanical extract optimization.

Collaborate with Ainnocence

Ainnocence is open to collaboration with academic groups, biotechnology companies, and industry partners interested in applying NatmolAI™ to natural-product-inspired discovery, molecular optimization, and complex chemical design challenges. The platform supports 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:
LinkedIn
YouTube

try to be careful about weeding out false and misleading content. As a user, if you see something we have missed, please do bring it to our attention. Your help is welcome. EIN Presswire, Everyone's Internet News Presswire™, tries to define some of the boundaries that are reasonable in today's world. Please see our Editorial Guidelines for more information.