AURIGENE.AI

Aurigene.AI: AI & Data powered DMTA cycle for faster and efficient drug development

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Key-highlights

- Aurigene.AI is a scalable, secure web-based cloud platform designed to accelerate the hit identification, hit-to-lead, and lead optimization process by reducing the DESIGN phase of Design Make Test Analyze **(DMTA)** cycle through an integrated artificial intelligence and physics-based simulation approach.
- The platform enables experts to design and prioritize the molecules based on **Generative-AI** and predictive **Multi-Parameter Optimization** (MPO) models enhanced with **Explainable-AI** capabilities and **Physics-based simulations.**
- The platform integrates structure normalization rules (SNRs) to ensure data quality and standardization while managing chemical and biological complexity, enabling the generation of chemically valid molecules for de novo design and predictive modeling.
- **Agentic AI** solutions for addressing drug discovery challenges and enabling efficient DMTA cycle execution through automation and intelligent decision-making.
- Aurigene.AI operates on five foundational pillars: data, models, compute, validation and collaboration.

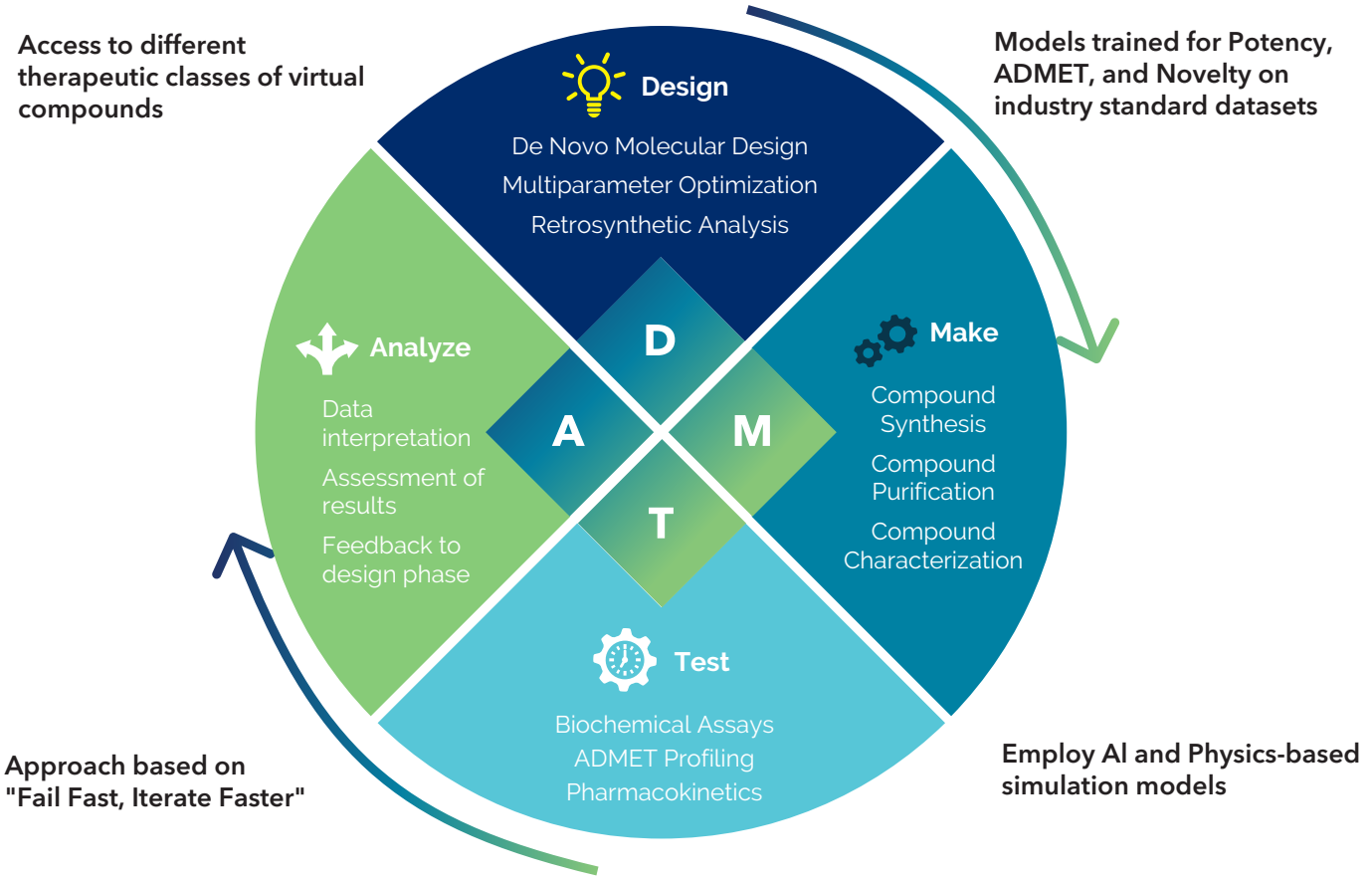
Tech-Driven Science

- **20+ Years of Expertise:** Backed by over two decades of scientific research and a dedicated team of experts.
- Robust Predictive Models: **Top-ranked** Absorption Distribution Metabolism Excretion and Toxicity **(ADMET)** models benchmarked with industry-standard datasets.
- Molecule ideation integrates **fragment growth, linker design, side-chain modification,** and **scaffold hopping,** complemented by structure-activity relationship (SAR) insights.
- Capable of handling multiple client projects ensuring project level **data segregation** and restricted cross project data contamination.
- Platform is powered by Nvidia's compute and secured infrastructure including encryption, **IAM controls, SOC compliance** and continuous monitoring.
- With Aurigene.AI, niche modalities such as peptides, proteins, DNA and RNA binders, targeted protein degraders (PROTACs and molecular glues), antibodies, antibody-drug conjugates (ADCs) and oligonucleotides are not a limitation.
- Giga-scale target focussed virtual screening on a chemical library of **3.5 Bn+** compounds.

Strength

- Highly experienced team with expertise to work in challenging projects in terms of complex targets that are otherwise difficult to understand using only conventional approaches.
- Proven real time success in offering AI/ML solutions for both **fast follower** and **novel target** use cases through an exhaustive POC study and client projects.
- The feedback mechanism enabled within the platform helps to fine-tune the existing MPO predictive models based on results from the experimental data, thus enables to refine the predictions and adapting to new targets or disease areas.

AI & Data-driven Design-Make-Test-Analyse (DMTA) cycle for drug development



Next-Gen Drug Discovery

- Real-World Validation: Proven success by handling multiple clients' projects having different problem statements focussed on designing patentable compounds, selective inhibition, controlled metal related metabolism.
- Scientific Rigor: Extensive experience working across a broad spectrum of targets.
- Computational Experimental Synergy: Integration of AI/ML and CADD predictions with experimental assays to confirm and prioritize high-potential drug candidates.
- Innovation Strategy: Proficient in managing multiple target product profiles for both fast follower strategies and first-in-class drug discovery initiatives.

Lab-in-Loop Validation

- Applied combination of Generative and Predictive AI along with the advanced physics-based simulation approaches.
- Identified hits with potencies ranging from 20 nM to 4 μM, each having distinct scaffolds and favorable ADMET properties.
- Design, synthesis and biological testing completed within a 3-month time period.
- Showcased rapid iteration using a fail-fast strategy.

Our offerings:

- Faster AI-driven IDD programs for novel or complex targets.
- Enrich discovery pipeline by generating novel and synthetically feasible compounds.
- Design novel inhibitors that act on primary targets while minimizing off-target effects.
- Address issues with potency and selectivity.
- AI-driven optimization of molecular ADMET profiles.
- A Target-focused virtual screening and compound synthesis.

Once with Aurigene, always with Aurigene! Our customers get a unique advantage of staying with us along the product lifecycle!

Scan this QR code to visit our website

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