VARIATIONAL AI

Generate novel, synthesizable small molecules tailored to your target product profile

Enki™ is a fully-trained generative AI foundation model built for small molecule drug discovery

Enki™ is a proprietary platform *purpose-built for drug discovery* - trained directly on molecular structures and properties from hundreds of millions of curated experimental and computational samples from 700+ drug targets. It produces compounds inherently optimized to meet your defined Target Product Profile.

Generate novel structures *de novo*
No reliance on known scaffolds or libraries.

Optimize properties simultaneously
Including potency, selectivity, ADMET, synthesizability, and more...

Work with minimal input data
Ideal for novel, data-sparse, or underexplored targets.

Fit your discovery workflow
Enki™ operates like a design-on-demand protocol, powered by generative AI.

How it works

1

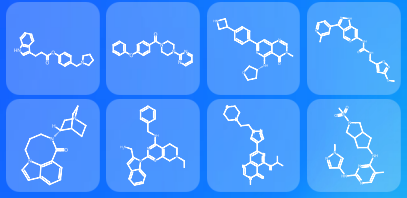
Define the preclinical target product profile (TPP)

Specify the On/Off-targets and physico-chemical properties of the molecules as input for Enki™ generative AI.

2

Enki™ generates compounds

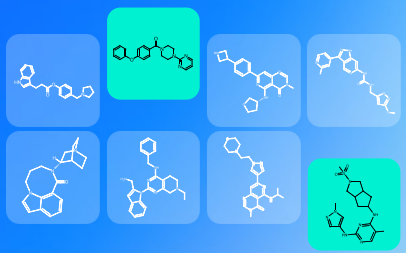
Enki™ generates novel and diverse structures that meet the defined TPP.



3

Make your selection

Pick compounds you want to synthesize and test.
Enki™ can also perform hyper-efficient lead optimization while constrained to a defined scaffold.



ENKI

Enki™ powers every stage of early discovery

Applied across Hit ID, Hit-to-Lead, and Lead Optimization, Enki™ adapts to the specific needs, data availability, and objectives of your discovery program.

Enki™ supports R&D teams throughout the early drug discovery process. From identifying novel hits to optimizing leads, Enki™ enables efficient exploration and refinement of small molecules at every key stage prior to preclinical development.

Use Enki™ to

Generate novel hit compounds that are diverse, synthetically accessible, and aligned with your project objectives.

Advance Hit-to-Lead progression with lead-like compounds optimized for potency, selectivity, and drug-likeness.

Streamline Lead Optimization with targeted improvements to key properties such as ADMET, selectivity, and potency.

Whether you're exploring low or no data targets or optimizing scaffolds for best in class targets, Enki™ integrates seamlessly into your discovery workflow - bringing generative AI to the earliest and most critical stages of small molecule drug discovery and development.

Trusted By

MERCK · RAKOVINA THERAPEUTICS INC. · ImmVue · ONCOCROSS

Additional undisclosed collaborations with public and private biotechs

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