

DESIGN YOUR NEXT MOLECULES WITH GENERATIVE AI

Artificial intelligence driven by chemistry

Forget about screening, START DESIGNING WITHIN MAKYA

Multi-parametric optimization from hit discovery to late-stage lead optimization

About Makya

Trained on 6 million patented organic reactions and powered by reinforcement learning, Makya explores a vast chemical space to design novel molecules with optimized properties, faster.

2,000+

Name reactions

1 Million

Building blocks

10²⁷

Molecules

ENHANCE YOUR CREATIVITY



Easy-to-use interface powered by AI



Diverse, novel & medchem-like molecules, on demand



Synthetic accessibility by design

SET YOUR CONSTRAINTS



3D Ligand-based & Structure-based modeling



SAR modeling

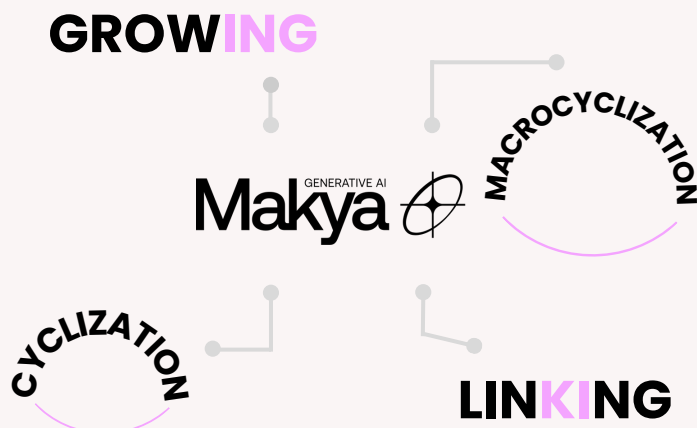


ADMET properties



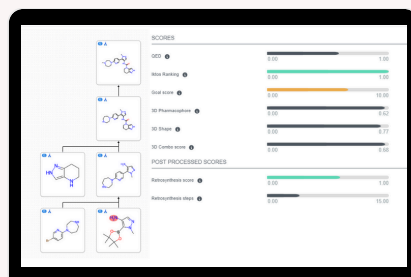
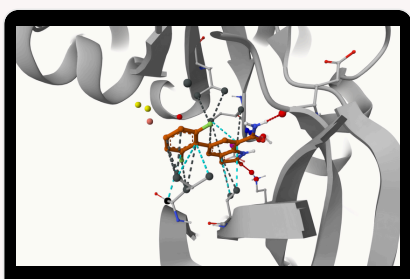
One Generative AI to address all use cases

From Hit discovery to Lead optimization



Makya enables **unprecedented exploration** of an ever growing chemical space, generating innovative and synthesizable molecules

01
Import PDB, SDF file, project data, define your Target Product Profile



02
Explore Generative AI capabilities with MPO, to discover novel and feasible molecules

03
Select ideal and optimized compounds, using all the scores: prediction, docking, shape, pharmacophore, etc...



CONNECTIVITY



Cloud based
Powered by AWS



API gateway

