

AIDDISON™ + SYNTHIA™ Software Integration

YOUR COMPLETE  
DRUG DESIGN TOOLKIT

Discover, optimize, and synthesize novel molecules in an integrated software ecosystem. AIDDISON™'s generative AI for de novo design meets SYNTHIA™'s retrosynthesis prowess, bridging the gap between virtual concepts and real-world chemistry.

## From Prediction to Pre-Clinical

Enhance your drug discovery workflows with seamless software solutions from target identification to synthesis, with the ability to quickly source starting materials from Sigma-Aldrich's world-class catalogs.



Lead  
Identification



Lead  
Optimization



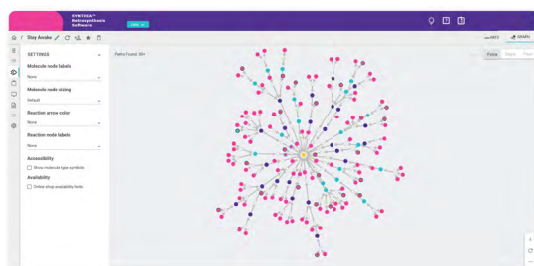
Retrosynthesis  
Planning



Optimization &  
Scale-Up

AIDDISON™ Software

SYNTHIA™ Software



Leveraging over 20 years of pharmaceutical research data, the AI-powered **AIDDISON™ platform** combines generative design, predictive insights, and 3D modeling in a turnkey solution for accelerated drug discovery.

- **Generate ideas** with rapid in silico screening of vast chemical databases and de novo design.
- **Optimize results** for synthesizability and ADMET properties with real-world ML models.
- **Evaluate and prioritize hits** with advanced data visualization and molecular binding tools.

Expert-coded by chemists and engineered by computer scientists, **SYNTHIA™ Retrosynthesis Software** allows scientists to quickly discover novel pathways for new and published target molecules.

- **Simplify route design** and quickly scan hundreds of pathways to find the best solution.
- **Reduce costs and save time** with the most cost-effective routes, state-of-the-art visualization and customization options meeting your project demands.
- **Generate new ideas and IP** by exploring unique and innovative syntheses for building your desired molecule.



Unlock your ingenuity and learn more  
about **AIDDISON**

See our webpage for further information,  
or contact us at [aiddison@milliporesigma.com](mailto:aiddison@milliporesigma.com)



Pioneer Your Pathway at  
**SynthiaOnline.com**



The Life Science business of Merck operates as MilliporeSigma in the U.S. and Canada.

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The secure cloud infrastructure is ISO 27001-certified and scalable for cost-efficient, seamless access.