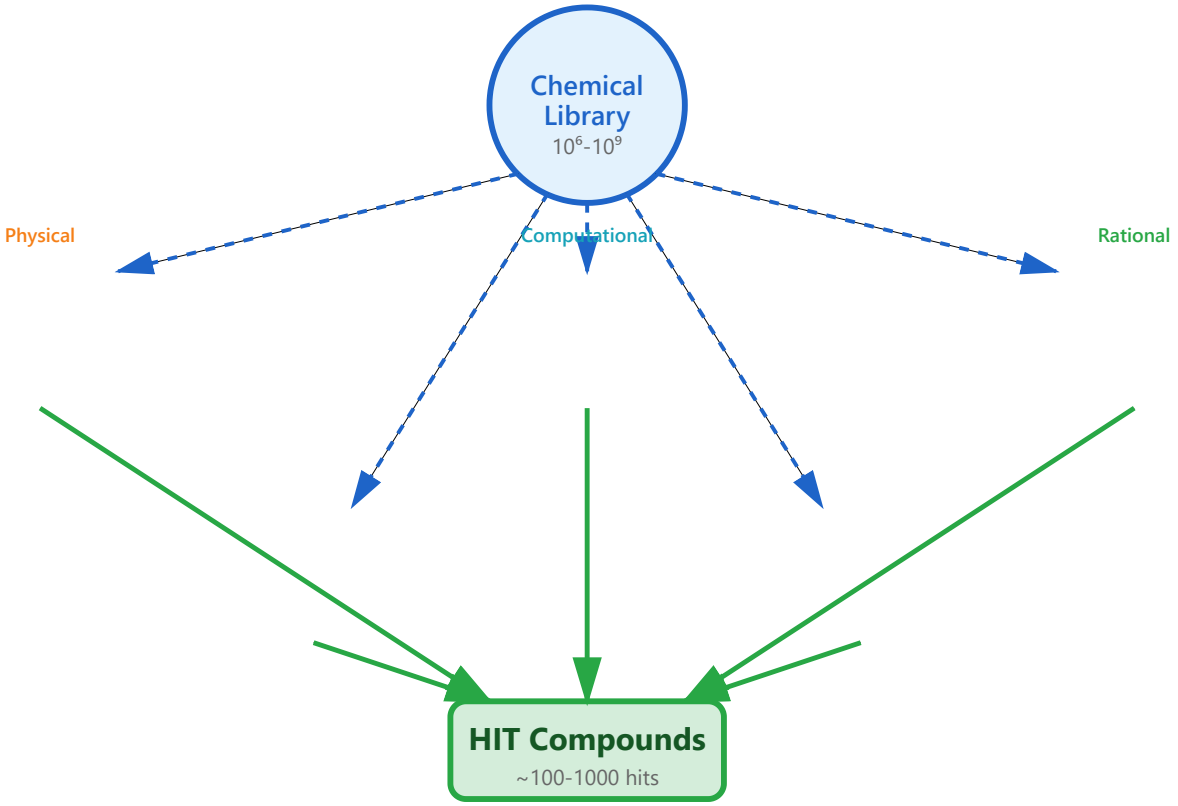
Lead Discovery



Methodology Principles

High-throughput Screening (HTS)

Uses robotic automation systems to rapidly test thousands to millions of compounds. Measures activity in parallel processing using 96, 384, or 1536-well plates to generate large amounts of data in a short time.

Virtual Screening

Predicts compound-target interactions through computer simulations. Selects promising candidates before experiments through molecular docking, pharmacokinetic prediction, and ADMET filtering to reduce cost and time.

🧩 Fragment-based Design

Binds small molecular fragments (MW < 300) to targets, then links or extends fragments based on structural information (X-ray, NMR) to grow them into optimized lead compounds.

🌿 Natural Products

Screens compounds derived from nature including plants, microorganisms, and marine life. Provides evolutionarily validated bioactive structures and offers inspiration for new drug development with unique chemical scaffolds.

🎨 Diversity Libraries

Compound libraries designed to cover chemical space as broadly as possible. Composed of compounds with diverse scaffolds, functional groups, and physicochemical properties to increase the probability of discovering unexpected activities.