Ligand Design™

What is Ligand Design™?
Cyclica’s Ligand Design technology generates new compounds with desirable multi-targeted profiles and advanced drug-like properties using a patented, evolutionary algorithm. Ligand Design digitizes the Design, Make, Test, and Analyze (DMTA) cycle traditionally carried out experimentally to rapidly design advanced drug-like molecules to accelerate your drug development programs.

What are the key features of Ligand Design™?
Generate novel compounds: physicochemical property filters and a generative algorithm encoded with retrosynthetic rules ensure compounds are drug-like and synthetically feasible

Prioritize compounds using the POEM predictive engine: Cyclica’s new machine learning algorithm predicts ADMET properties from chemical structure alone

Assess protein-ligand interactions through the MatchMaker™ Engine: Cyclica’s proprietary deep learning algorithm assesses the compatibility between compounds and designated protein targets

Evolve compounds over multiple generations: an evolutionary metaheuristic algorithm and advanced scoring functions select top compounds from each generation to engineer desired functionality

Incredibly fast predictions: explore synthetically accessible chemical space (~10^60), assess millions of potential compounds, and return a manageable collection of promising drug-like compounds in just 2 days.

Easy Workflow
1. Select proteins for your protein panel (targets/anti-targets)
2. Provide seed molecules (eg. known binders, endogenous ligands, FDA-approved drugs) as the starting point
3. Specify the physicochemical and ADMET properties desired for your new drug candidates
4. Generate a collection of novel multi-targeted drug-like molecules with desirable polypharmacology and molecular properties for synthesis
5. Receive expert support from Cyclica’s Applied Scientists throughout the course of the project