molecular forecaster

MAKE SMARTER DECISIONS IN DRUG DESIGN

Molecular Forecaster Inc. (MFI) is advancing small molecule drug discovery, with human expertise, proprietary software that works like a partner, and an all-in approach to collaboration that sets customers up for success.

WHAT WE DO

HIT IDENTIFICATION

Identify promising drug candidates from complex chemical spaces to accelerate early-stage discoveries.

HIT-TO-LEAD

Refine hits into drug-like candidates, optimizing their properties to ensure stronger, more selective molecules for further development.

LEAD OPTIMIZATION

Optimize lead candidates, to enhance efficacy, minimize toxicity, and ensure the best possible pharmacokinetic profile for clinical success.

UNIQUE FEATURES OF THE FORECASTER PLATFORM

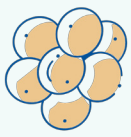
Niche solutions: including covalent drug design and targeting of metalloenzymes or RNA

CYP450 metabolism: prediction of CYP oxidation, inhibition, and induction

Virtual chemical library design: chemistry-centric tools for SAR, clustering, and custom library creation

OTHER SCIENCE BEHIND THE SERVICE WE OFFER

STRUCTURE-BASED DESIGN



MOLECULAR DYNAMICS

LIGAND-BASED DESIGN

CHEMOINFORMATICS AND MACHINE LEARNING

QUANTUM MECHANICS

WHO WE WORK WITH

START UPS	FLOURISHING BIOTECHS OR CROS	ACCELERATORS, INCUBATORS, AND INVESTORS	ESTABLISHED PHARMA

WORK WITH US

Fee-for-service or full-time equivalent **service-based model**

- No IP claims, you retain full ownership
- No internal pipeline, we're fully focused on helping you, not launching our own assets
- Flexible working models based on your pipeline needs

License Forecaster **SaaS-based model**

- Local or cloud installation with dedicated technical support
- No usage restrictions, full access to all licensed modules
- Unlimited users per location; no tokens, no overage charges, no hidden fees

YOUR CHALLENGES, OUR SOLUTIONS

You've got a capable team but lack internal capacity or know-how.

Create complementary bandwidth with MFI's cross-functional team of computational, medicinal, and synthetic chemists.

You need more chemistry expertise in your computational contribution.

Access specialized knowledge and expertise to optimize compounds and accelerate drug design progress.

Your off-the-shelf software doesn't meet the demands of your projects.

Use software designed for flexibility, adaptability, and evolution to meet unique project objectives.

You want to outsource administratively, but maintain strong internal alignment.

Collaborate with a team as focused as you on making smart, strategic decisions.

Let's talk about how we can support your drug design projects.

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Molecular Forecaster Inc. (MFI) helps organizations make smarter decisions in drug design. We've spent six years democratizing computer-aided drug design via our highly collaborative research-as-a-service model. Today, we're integrating what we've learned into new and improved software tools. Our goal? To become the go-to partner in small molecule drug design, combining proprietary tools and technology, our expertise and know-how, and our all-in approach to collaboration that sets our partners up for success.