INTEGRATED DRUG DISCOVERY

Target Analysis

Molecular biology
Protein production
PPI modulation

Hit Identification

Assay development
HTS, Fragment-based approaches, DEL-ML-CS
Giga-scale - ML- assisted virtual screening
ML- accelerated mmPBSA/FEP

Hit Expansion

2D/3D QSAR
Similarity searches
(FTrees, SpaceLight, SpaceMACS)
Generative AI
Pharmacophore modeling

Hit-to-Lead

Computer-aided drug design
Medicinal chemistry support
Custom library design and synthesis
ADME profiling

Lead Optimization

Full support on DMTA Cycle
Custom library design and synthesis
In vitro and in-vivo DMPK

Preclinical Studies

Safety Profiling
Synthetic optimization of candidates, scale-up
Metabolic and impurity identification
and synthesis

Benefits work with us?

- ✓ Efficient management of your projects
- ✓ CADD, synthesis and biology working simultaniously on your problem
- ✓ Access to the largest compound colelctions and efficient search algorithms: Enamine xREAL, Freedom Space, in-stock collection
- ✓ Skilled multidisciplinary team: chemistry, biology, CADD, medicinal chemistry

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chem-space.com

We employs and connect scientists' expertise in Medicinal Chemistry, Synthetic Chemistry, Computational Chemistry, AI/ML, Molecular Biology, Structural Biology, and Bioanalytics to deliver the drug candidates fast and efficiently.

Hit Finding

- Machine Learning (ML)-supervised
- DNA-encoded library processing
- Giga-scale virtual screening utilizing the V-SYNTHES
- ML-boosted giga-scale docking

Research Infomatics

- Structure-based and ligand-based virtual screening
- Molecular dynamics simulation
- ML-based services: data analysis, hit expansion, DiffDock, properties
- prediction, active learning
- Fragment-based drug discovery

DESIGN

The Largest Catalog

- 300,000 building blocks in-stock
- 4.4M in-stock screening compounds
- Liquid stock collection of 800K+ compounds
- Over 60 ready-to-deliver pre-plated libraries

REAL Compounds

- 70B REadily AccessibLe compounds
- 3-4 weeks turnaround time
- Over 80% synthesis success rate

Chemical Services

- Diverse bench chemistry
- Developmemt of custom libraries
- Compound management services
- Over 800 skillful synthetic chemists

MAKE

Molecular Screenning

- Cell biology
- High Throughput Screening
- Secondary assays: surface plasmon resonance, high content screening, western blot analysis

Bioanalytics and *In vivo*

- Formulation studies
- Pharmacokinetics in rodents
- ADME, toxicity

Protein Production

- Protein expression in bacterial, mammalian, and baculovirus systems
- protein purification
- Bacterial screens

TEST

ANALYZE

- Batch comparison
- Analysis of obtained data
- AI/ML model development
- Structure-activity relationship (SAR)
- Creation of custom chemical spaces based on obtained data
- Formulate hypothesis and provide you with comprehensive reports