Integrated Drug Discovery Services

CHEMSPACE
Delivering Discovery Solutions®

Target Analysis

Molecular Biology
Protein Production
PPI Modulation

Hit Identification

Assay Development
(cell-based, biochemical, biophysical)
HTS, Fragment Screening, DEL-ML-CS
Giga-scale-ML-assisted Virtual Screening

Hit Expansion, SAR by catalog

ML-assisted SAR, 2D/3D QSAR
3D Pharmacophore Similarity
Steered MD

Hit-to-Lead

Computer-aided Drug Design
Generative AL
Custom Library Design and Synthesis
ADME Profiling

Lead Optimization

Holistic Design
Accelerated 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 synthesis

Design

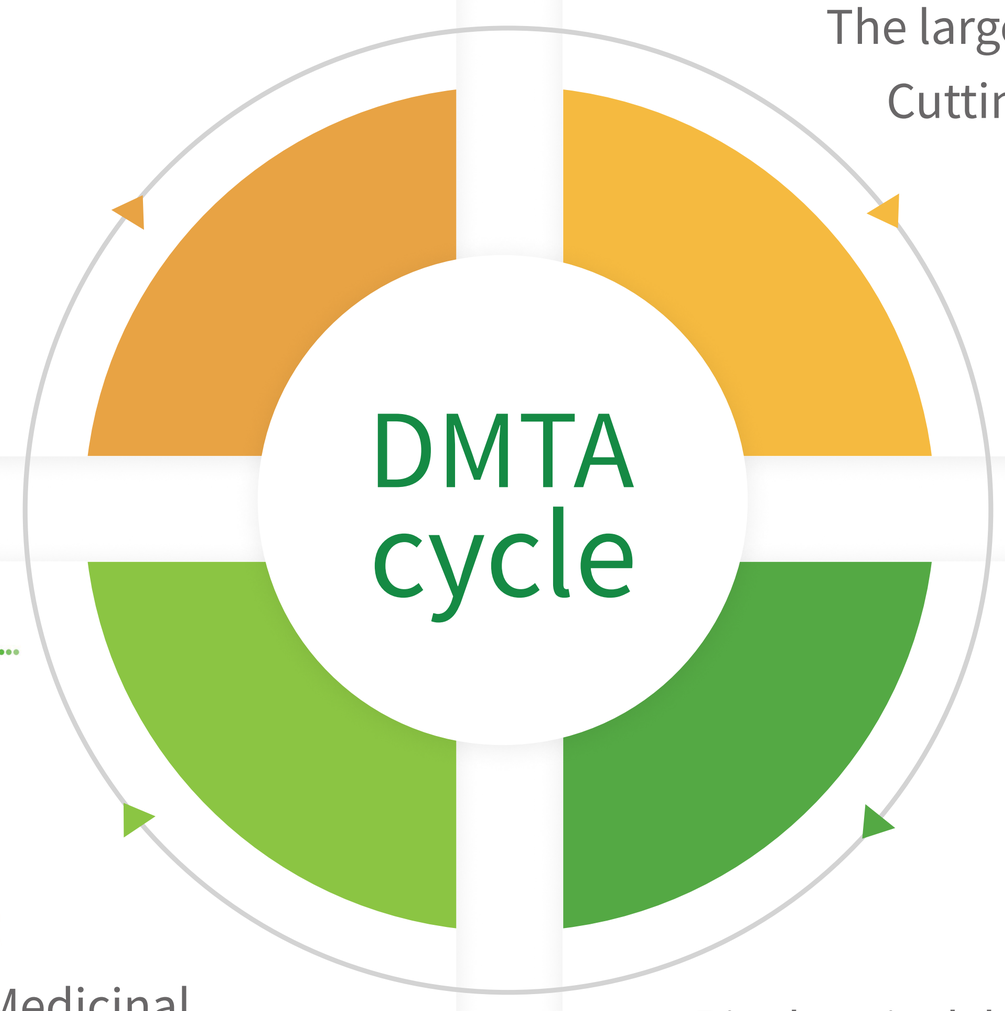
Medicinal/Computational Chemistry, AI/ML

Holistic design
CADD/QSAR
ML-modeling
Generative AI

Make

Synthetic Chemistry

The largest Stock of BBs and reagents
Cutting-edge synthesis technology
Billions of MADE compounds
Parallel chemistry



Analyze

Program Management

The joint team of experts in Medicinal chemistry, computational chemistry, AI/ML, data science to analyze and interpret the results

Test

Biology

Biochemical, biophysical, cell-based assays
In vitro and in-vivo DMPK
ADMET

Why CHOOSE US?

Efficient Project Management: We handle all aspects related to the management and implementation of your project.

High-Skilled Team Collaboration: Benefit from the expertise of a highly skilled team comprising professionals from Enamine, Chemspace, and Bienta.

Largest Collection Access: We provide access to extensive collections of building blocks and screening compounds, empowering efficient drug discovery efforts.

Unique approaches to giga-scale chemical space exploration. Benefit from rapid and efficient hit finding, hit expansion, and SAR analysis within chemically accessible spaces: Enamine xREAL (2.7T) and Freedom Space 3.0 (5B).

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