X-CHEM
TAKE THE LEAD. DRIVE DISCOVERY.

HITMiner®

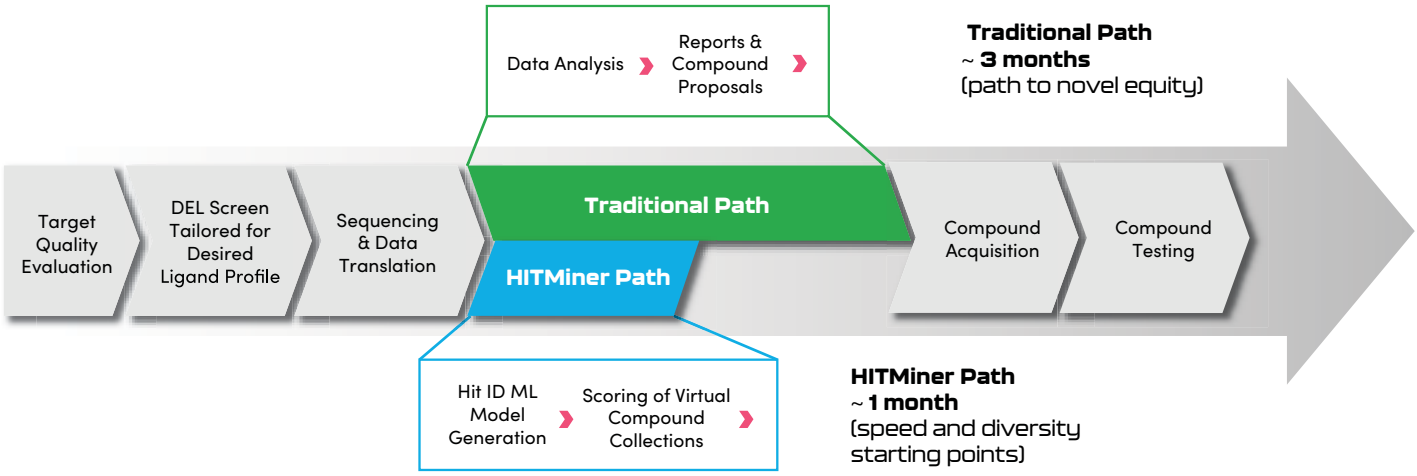
Quickly Expand Diversity of Hits With Novel Chemistry

Machine Learning (ML) can only be powerful if the training data is of good quality. With HITMiner, we leverage our impeccably diverse library decks and robust informatics pipeline to transform experimental measurements from billions of compounds into rich datasets. Using these expert-curated datasets as the training data for our multi-representation hub—ArtemisAI, our partners can attain series of chemically diverse series from virtual catalogs of their choice to jumpstart their campaigns.

HITMiner

Broaden hit identification for even the most challenging targets with our DEL and computational experts through high-quality DEL data from billions of compounds synergized with advanced ML models.

Explore far more diverse and readily accessible chemical space with shortened discovery process



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Our proven impact:

Machine learning on DNA-encoded libraries: A new paradigm for hit-finding (in collaboration with Google Research)

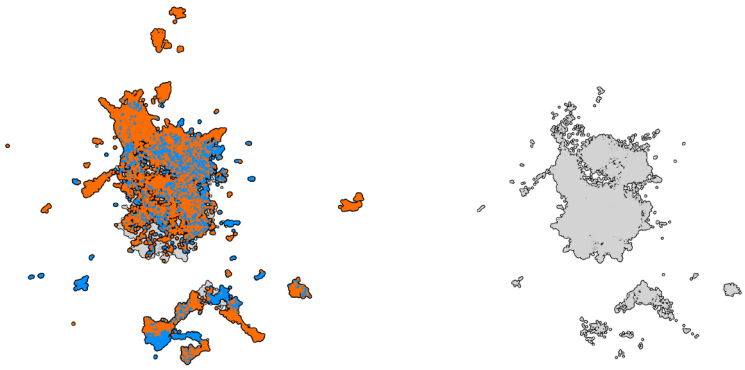
We developed the first effective ML platform based on DEL selection data. The platform predicted highly potent small molecule inhibitors within a virtual library of commercial compounds across diverse protein targets.

Discovery of a First-in-Class Small-Molecule Ligand for WDR91 Using DNA-Encoded Chemical Library Selection Followed by Machine Learning

Our approach of ML on DEL data predicts a novel selective tool compound and covalent analogues to evaluate WDR91's therapeutic potential.

High-quality Data and Diversity Are Top Priorities

X-Chem's library mirrors the vast virtual space of drug-like and lead-like chemical compounds. Every DEL screen as part of a HITMiner project yields massive amount of diverse, biologically relevant data annotated with specific binding measurements, which are a key foundation to building our machine learning algorithms. For partners seeking to access readily purchasable compounds quickly, HITMiner can confidently make inferences on molecules from commercial catalogs (or their own catalogs), thanks to the wide coverage of chemical space in our high-quality training data.



Chemical diversity plots showing an equal number of compounds of X-Chem libraries overlaid onto Enamine REAL (left), and Enamine REAL only (right).

The HITMiner Advantages

Within the three-month process of HITMiner, inclusive of DEL screen:

- Our DEL, medicinal chemistry and and ML experts collaborate with you on every step of your project.
- We ensure the best reagent quality and screen design.
- We tailor our screening and ML-training to your target.
- We review and validate the identification, novel hit recommendation from any virtual catalog.
- You save on synthesis costs, shorten your hit-finding timelines and expand the diversity of chemical hits.

Discover the Power of HITMiner

ABOUT X-CHEM

X-Chem, Inc. is the leader in small molecule discovery science, providing pharmaceutical and biotech companies a complete, seamless solution for screening, hit validation and lead optimization. As pioneers of DNA-encoded chemical library (DEL) technology, the company leverages its market-leading DEL platform to discover novel small molecule leads against challenging, high-value therapeutic targets. In-house lead optimization services enable clients to progress their compounds directly for even higher quality outputs. Our expertise in medicinal chemistry, custom synthesis and scale-up process chemistry enables us to support all aspects of drug discovery, supporting lead optimization through candidate identification.

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