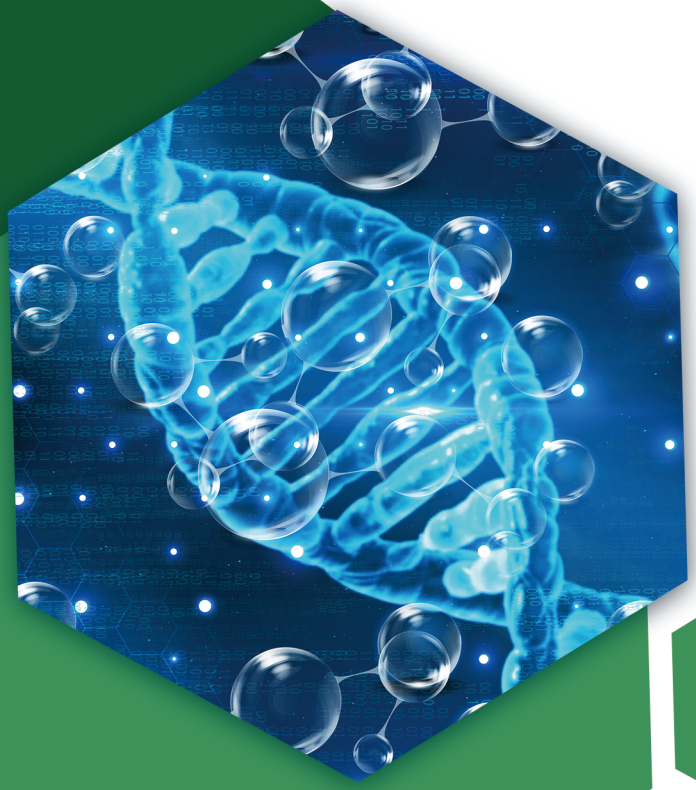
药明康德
WuXi AppTec

DELopen

HANDBOOK



DELopen Website

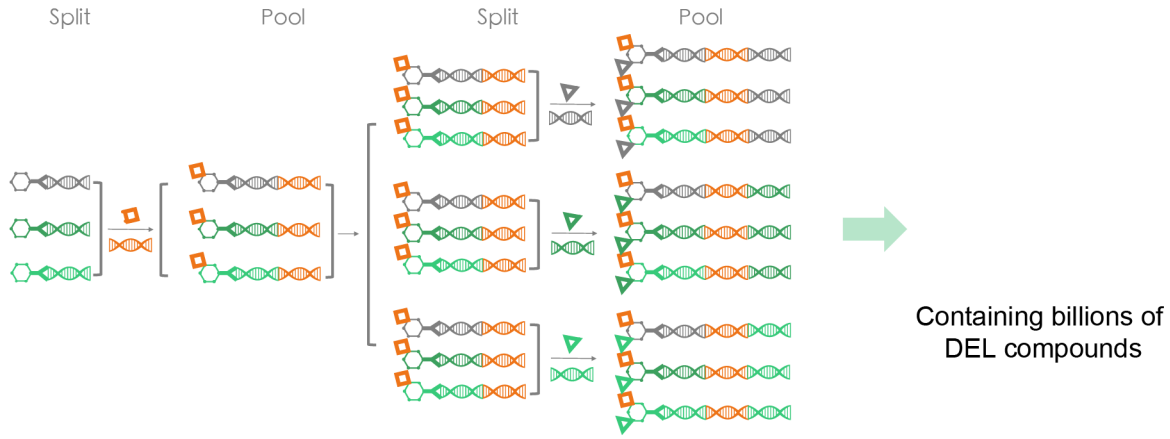
HitS Website

An elegant approach for drug discovery

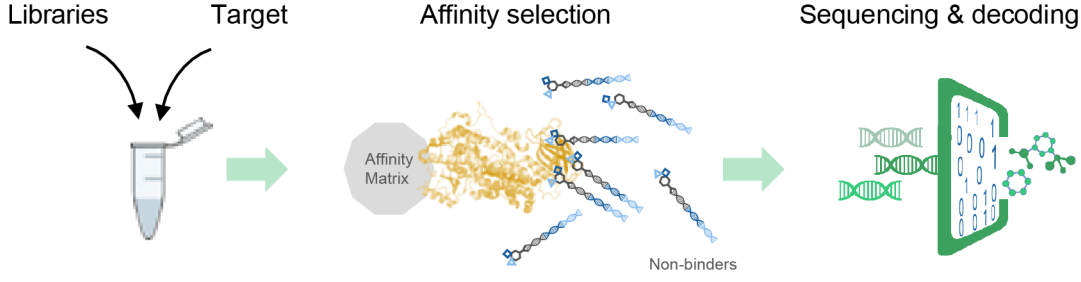
DNA-encoded library (DEL) is a technology that enables fast screening of billions of small molecule compounds in early phase of drug discovery. The aim of DEL technology is to discover novel chemical structures for validation and optimization.

A three-cycle DEL compound

DEL enables mass creation of chemical libraries by a combinatorial chemistry approach, namely Split & Pool.



DEL makes it possible to screen billions of compounds in a small tube. Thanks to high-throughput sequencing technology, compounds can be uniquely identified by their DNA barcodes.



Introduction

DELopen provides free access to DNA-encoded libraries (DEL) for academic users and encourages an open, community-based approach to data sharing.

Free access

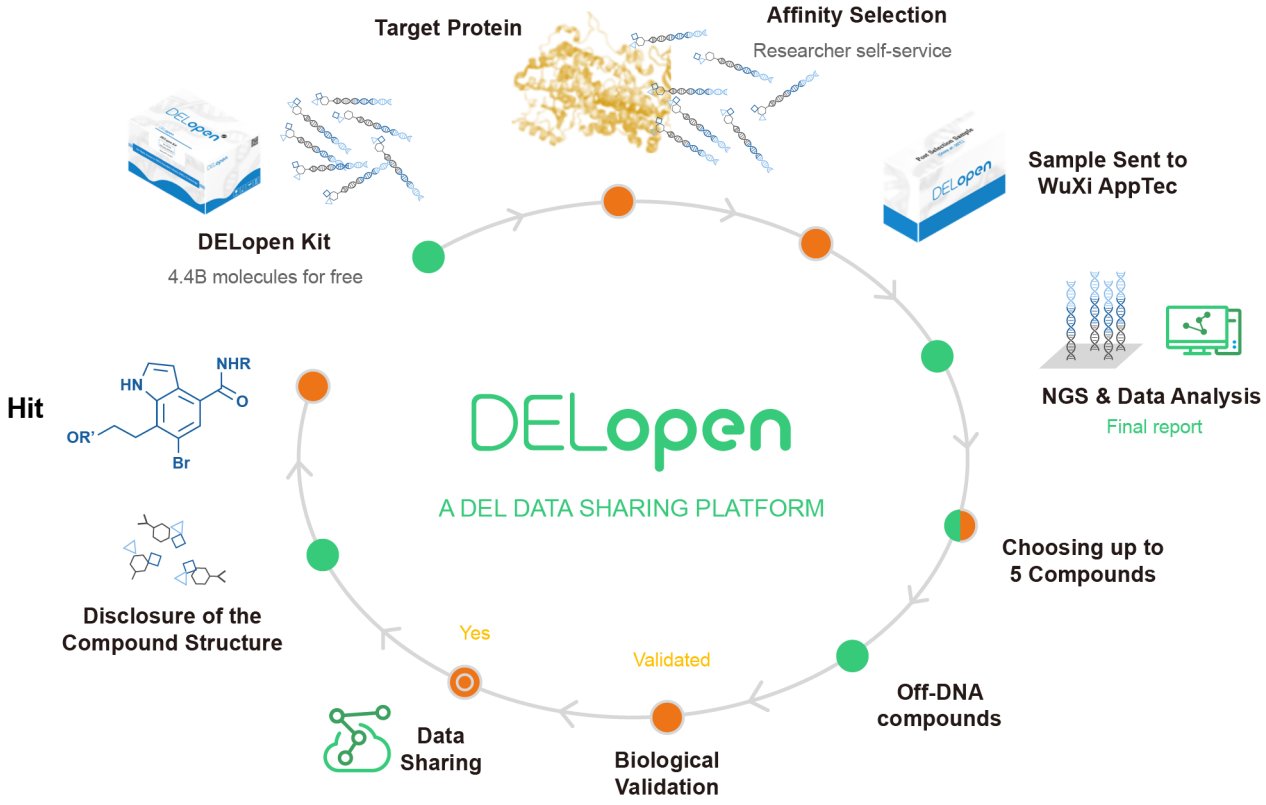
Data sharing

Compatible with computational tools

Well-balanced chemical space

DELopen users are able to conduct affinity selection experiments in their own labs, and WuXi AppTec HitS is responsible for post-selection processing, sequencing and data analysis.

If promising hits are identified and validated, users can choose to disclose their target in exchange for the chemical structures.



DELopen Scientific Advisory Board

DELopen platform is dedicated to the development and application of DEL technology in drug discovery, initiated by WuXi AppTec in conjunction with leading academic researchers.

With the support provided in this partnership we aim to bridge academia and industry and jointly promote the application of DEL technology in the field of new drug discovery.

—— Richard Lerner
The Scientific Advisory Board chairman for DELopen

Roger Kornberg
Stanford University

David R. Liu
Broad Institute

Phil Baran
Scripps Research

Carolyn Bertozzi
Stanford University

Raymond Dwek
University of Oxford

Chi-Huey Wong
Scripps Research

Richard Soll
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Weill Cornell Medical College

Casey J. Krusemark
Purdue University

K. Barry Sharpless
Scripps Research

Alan Saghatelian
Salk Institute

Mark Yeager
University of Virginia School of Medicine

What users say

Jia Xie Ph.D.

Investigator at Scripps Research
Assistant Professor University of Miami

I would highly recommend people to try it out. I wish the program can grow bigger and better, helping to promote basic research from a never-before-seen angle.

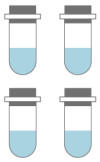
Erkan Baloglu Ph.D.

Founder and Principal at Boston Biotech Consulting

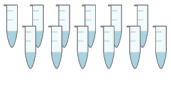
The DELopen screen procedures were very straight forward. And two highly experienced WuXi AppTec scientists were there with us through the procedures and answered any questions we might have.

What is included in DELopen service

DELopen kit



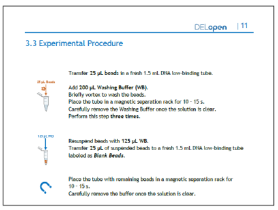
- DELopen libraries×4 (30 libraries, 4.4 billion compounds)
  For 4 experimental conditions



- Post-selection sample empty tube×12
  For sending samples to WuXi AppTec

- Sheared salmon sperm DNA solution
- 10×PBS buffer containing 0.5% Tween 20
  For preparing washing buffer and selection buffer

Technical support



User manual with step-by-step instructions

Tutorial videos on affinity selection

DELopen teaching lab in Boston and Munich

Service included

Post-selection processing	▪ Sample quantitation by qPCR ▪ PCR amplification
Sequencing	▪ Next generation sequencing (NGS)
Data analysis & online platform	▪ Decoding ▪ Filter setting ▪ Online data visualization platform

Fee-for -service

DELopen users can choose to synthesize the corresponding off-DNA compounds at WuXi AppTec.

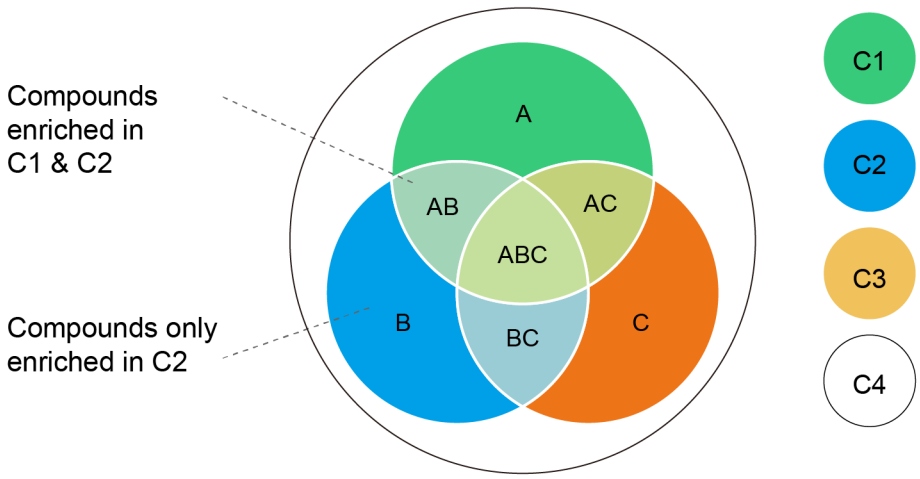
What to prepare for a DELopen screen

Experimental design

Experimental designs that are commonly used for DELopen:

- Different types of proteins
- Domains or mutations of interest
- Protein samples plus additional reagents, such as inhibitors

#	1	2	3	4
Condition	Protein 1	Protein 1 + Inhibitor	Protein 1_D1	NTC
Purpose	Main target	To block a pocket	Domain of interest	To remove background noise



Protein & affinity matrix

Requirements for protein:

- Having certain tags for immobilization
- Pure, homogenous, and properly folded

Requirements for affinity matrix:

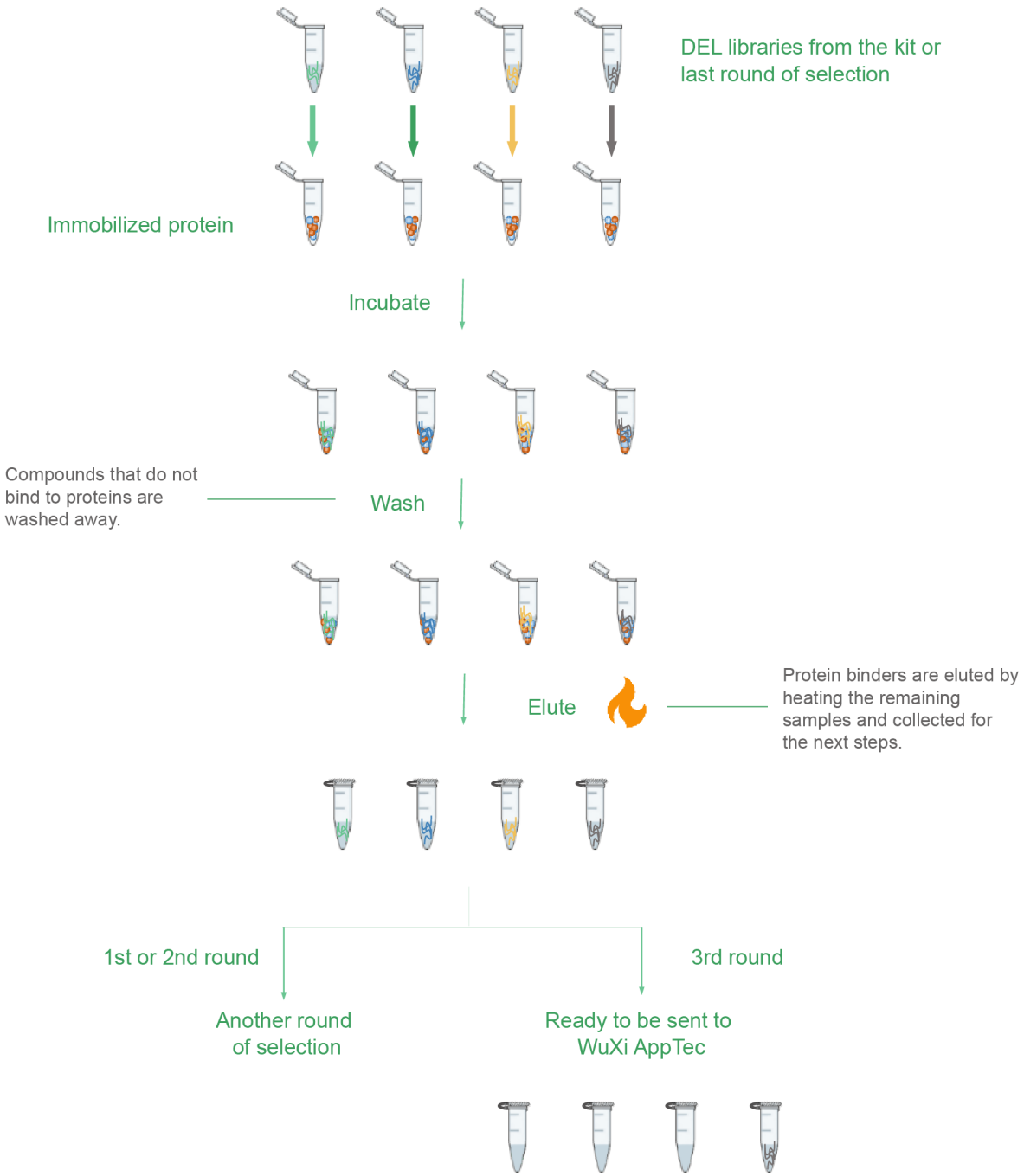
- Compatible with protein tags
- Magnetic beads are recommended, such as HisPur™ Ni-NTA Magnetic Beads
- Protein capture test is needed prior to affinity selection

Lab Equipments

- PCR system
- Gel electrophoresis & imaging system
- Microcentrifuges
- Rotators
- Heaters

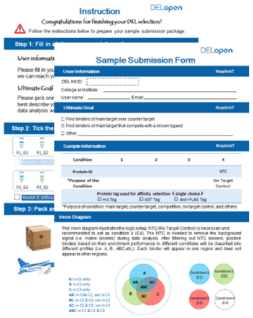
Affinity selection

Typically, three rounds of affinity selection are needed to reach the desired quality of selection samples.



When affinity selection is completed

Shipping samples



Fill in the sample submission form.

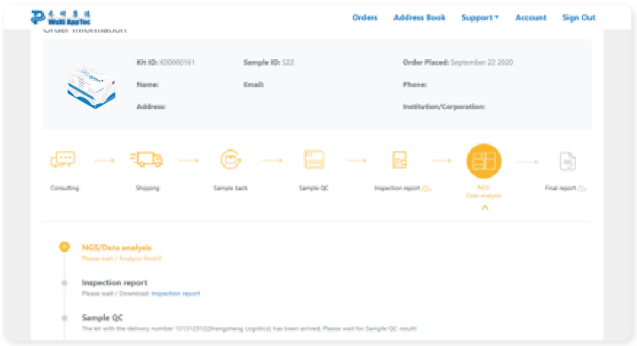
Store samples at -80℃ or on dry ice until shipment.

Ship with dry ice to WuXi AppTec at Shanghai, Boston or Munich.

Online tracking

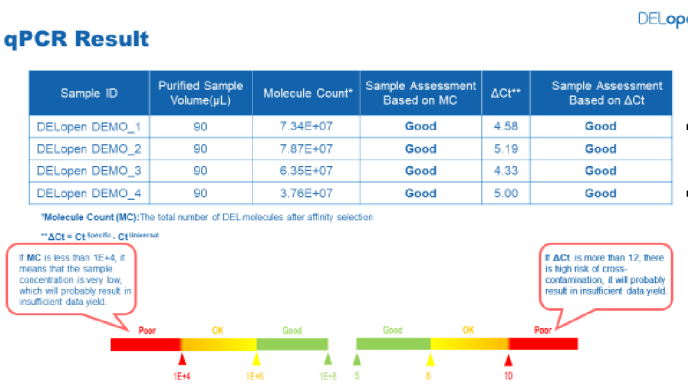
DELopen users can track the progress of their samples through an online portal.

Website: https://hits.wuxiaptec.com



Inspection report

Inspection report is provided for users based on post-selection processing results.

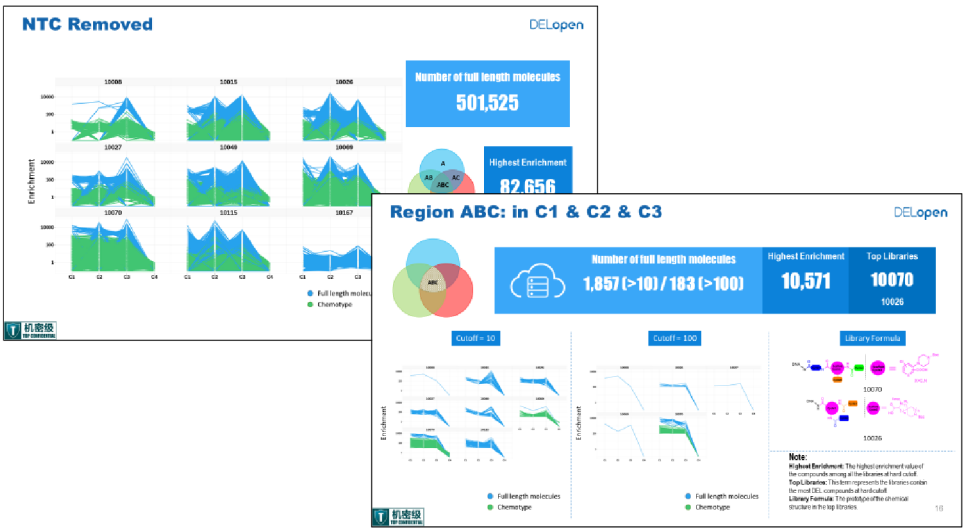


- The amount of DEL compounds
- Evaluation of contamination

Understanding DELopen screening data

Final report

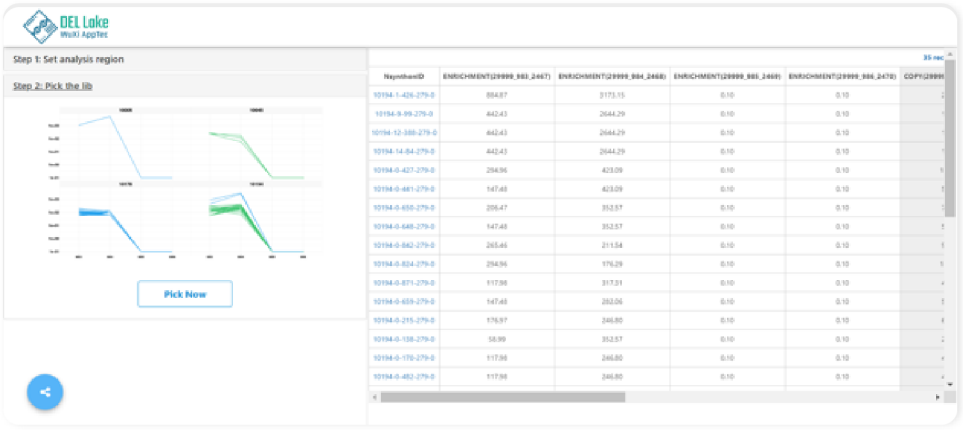
- Motif analysis to detect possible DNA binding sites of the target protein
- Enrichment of compounds and chemotypes across different conditions

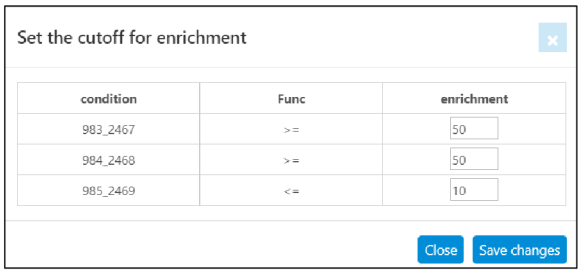


Interacting with data

Online platform for users to interact with copy numbers and enrichment scores

Website: https://hits.wuxiapptec.com



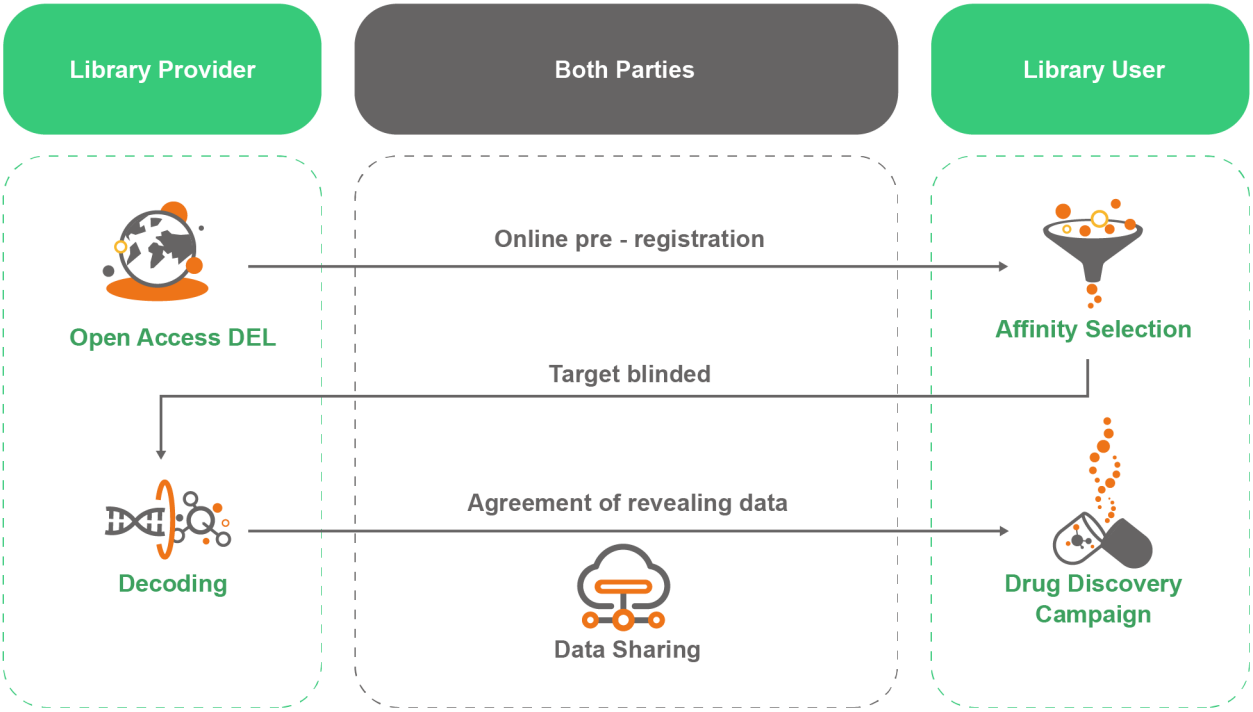


- Customizing data analysis

- Looking into specific DEL libraries

Data sharing & exchanging for structures

If identified hits are validated by certain biological assays, users can choose to share information of their experiments in exchange for associated chemical structures.



Data deposits obtained from DELopen users will go to a database established for data mining and developing novel applications of DEL.

What to share

- Target information
- Results of biological validation

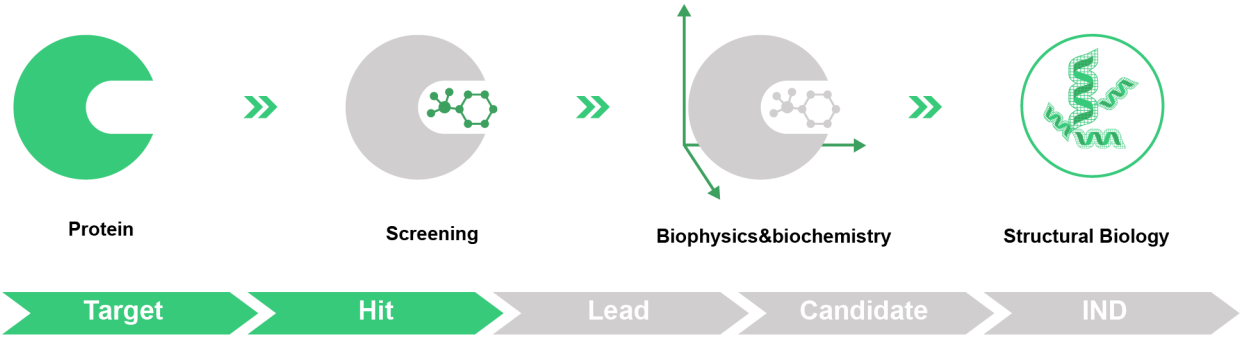
Potential benefits for community

- A DEL database with historical screening information
- Annotation of libraries for a given class of targets
- Systematic annotation of on target/off target effects
- Screening a pathway or a group of proteins
- For you to unlock other research possibilities

WuXi AppTec HitS

The industry-leading Target-to-Hit platform at WuXi AppTec HitS unit facilitates protein production, hit identification, biophysics and structural biology to accelerate drug discovery.

With operations and expert team located in China, Europe and North America, we proudly support pharmaceutical companies, biotech firms and academic researchers from all around the world.



HitS has an integrated team of experts in DEL screening, who specialize in chemistry, biology, bioinformatics and data analytics.

Our mission is to bring DEL service of high quality to drug developers by providing flexible business models and customized screening strategies.

DELpro

One-stop solution customizable

46+ Billion

Target exclusivity
For all drug developers
Access to unigue scaffolds

DELight

Unprecedented data release

15.1 Billion

Target confidentiality
For all drug developers
Easy access with reduced risk

DELopen

Free access to DEL, data sharing

4.4 Billion

Target confidentiality
For academic users
Open source

HitS Website: https://hits.wuxiapptec.com
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North America: Declan Ryan declan.ryan@wuxiapptec.com
Europe: Dave Madge dave_madge@wuxiapptec.com

DELopen Website

HitS Website

Contact information:

Pre-registration for Free compound library via DELopen:

https://www.delopen.org

More information about products and solutions:

https://hits.wuxiapptec.com