A New Method of Hit Discovery

In contrast to high throughput screening, DEL requires a very small amount of target protein and minimum assay development. More importantly, it disrupts the concept of “cost-per-well” and allows testing billions of compounds in one tube.

Warhead DNA barcode

Affinity selection

Sequencing & decoding the binders

Allowing access to more chemical space with lower cost

Novel Business Model — Three Types of Services Designed For Different Needs

4.2 Billion

DELopen

Free access to DEL data sharing

Target confidentiality For academic users
Open source

10.8 Billion

DELight

Unprecedented data release

Target confidentiality For all drug developers
Easy access with reduced risk

41+ Billion

DELpro

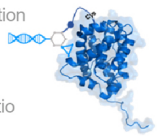
One- stop solution customizable

Target exclusivity For all drug developers
Access to unique scaffolds

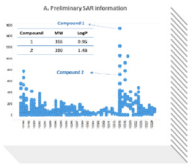
Extended Research Field — More Than Conventional DEL Screening

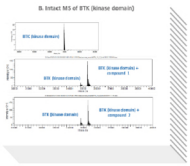
Irreversible Covalent Screening

Specially designed library collection with **electrophilic warheads**



Optimized selection method to enhance the **signal-to-noise** ratio

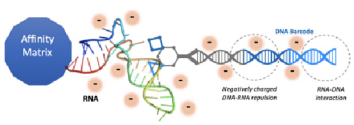




Pre-incubation Time (h)	Cmpd 1 IC_{50} (nM)	Cmpd 2 IC_{50} (nM)	Ibrutinib IC_{50} (nM)
0	14	2,600	49
3	0.1	50	11

RNA Target

Optimized selection procedure to counter **charge, RNA/DNA interaction and structural integrity** of RNA during DEL screen

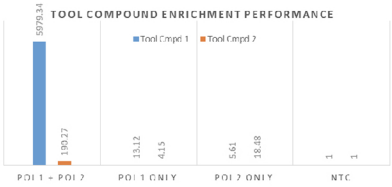


Compound	Library	SPR (K_D)
RNA Hit 5 & 6	3 cycle library	Strong binding
RNA Hit 7	2 cycle library	1.7 uM
RNA Hit 8	2 cycle library	1.3 uM
Reference	Positive Control	144 nM

PROTAC and Molecular Glue

Optimized selection method to specifically enrich **dual-binding** molecules

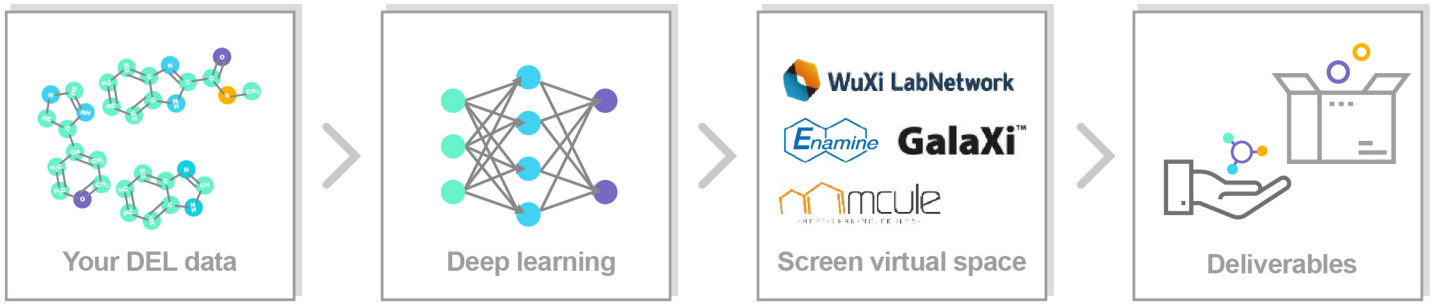
On-DNA Tool compound 1 binds to POI 1 & 2
On-DNA Tool compound 2 only binds to POI 2



WuXi AppTec HitS

药明康德
WuXi AppTec

DEL-enhanced Virtual Screening

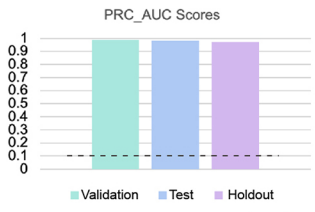


Data curation and assessment

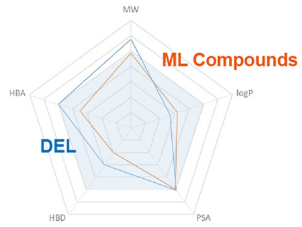
32,167

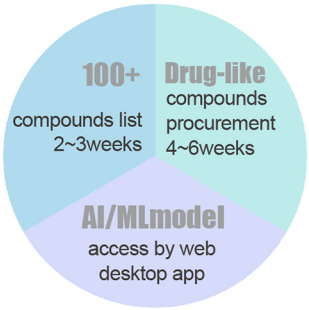
242,817

Model training and evaluation



Drug-like test compounds from commercially available catalogs





	DEL	Structure Based Virtual Screen	DEL + ML
Compound library	DNA-encoded compound	Virtual + Commercial library	Virtual + Commercial library
Selection method	Experimental	Computational	Computational
Protein structure	Not needed	Required	Not needed
Compound acquisition	Resynthesis	Off-the-shelf or Resynthesis	Off-the-shelf or Resynthesis
Screen time	4 weeks	3-4 weeks	2-3 weeks
Hit rate	5-50%*	1-25%**	5-32%

** In house statistics ** J. Med. Chem. 2013, 56, 17, 6560–6572*

Contact Us

PHONE
US:+1(857)500-0235
China:+86(021)2066-3521

EMAIL
HitS_service@wuxiapptec.com

WuXi AppTec HitS US
Suite 111,22 Strathmore Road Natick
MA 01760-2434,USA

Crelux GmbH, a WuXi AppTec Company
Am Klopferspitz 19a
82152 Martinsried,Germany

WuXi AppTec HitS China
240 Hedan Road,Shanghai 200131,China
1318 WuzhongAvenue,Suzhou 215104,China

Hits Website

WuXi AppTec HitS