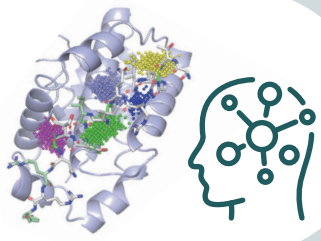
AXCELEAD
Drug Discovery Partners

Data-Driven High-Throughput Screening (HTS) Platform

The integrated HTS platform combines computational chemistry with AI/ML to maximize the efficiency and quality of hit identification.

Pharma-Origin High-Quality Compound Libraries



Maximized HTS Efficiency by Computational Chemistry & AI/ML

Comprehensive HTS Experience and Extensive Track Records

Pharma-Origin High-Quality Compound Libraries

Axcelead Proprietary Compound Library

>1.2 M compounds in stock

>1.2M
Compound library

Ready-to-use HTS Library

Diversity libraries

- Single library >333K compounds
- Pooled library >500K compounds (10 compounds mix in 1 well)
- Pooled library for ASMS >333K compounds (400 compounds mix in 1 well)

>333K
Single diversity HTS library

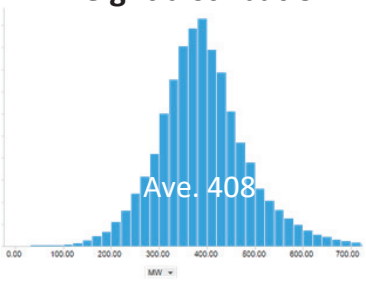
Focused libraries

- Chemical property-oriented library (fragment, CNS, extended Rule of 5)
- Target oriented library (Kinase, GPCR, PPI, RNA, nuclear receptor, etc.)
- RNA targeting small molecule library (RNA binders, splicing)
- Molecular glue degrader library (CRBN, DCAF15, E3 etc.)
- Biological annotation (FDA-approved, proprietary assay database etc.)
- Covalent & chemical proteomics (cysteine-focused)

>500K
Pooled diversity HTS library

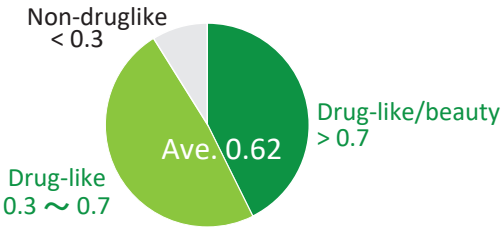
High quality compound library

Diversity of molecular weight distribution

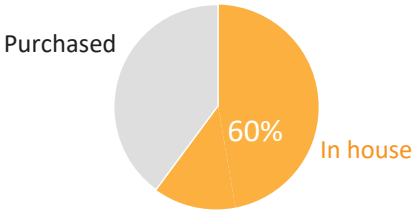


High drug-likeness

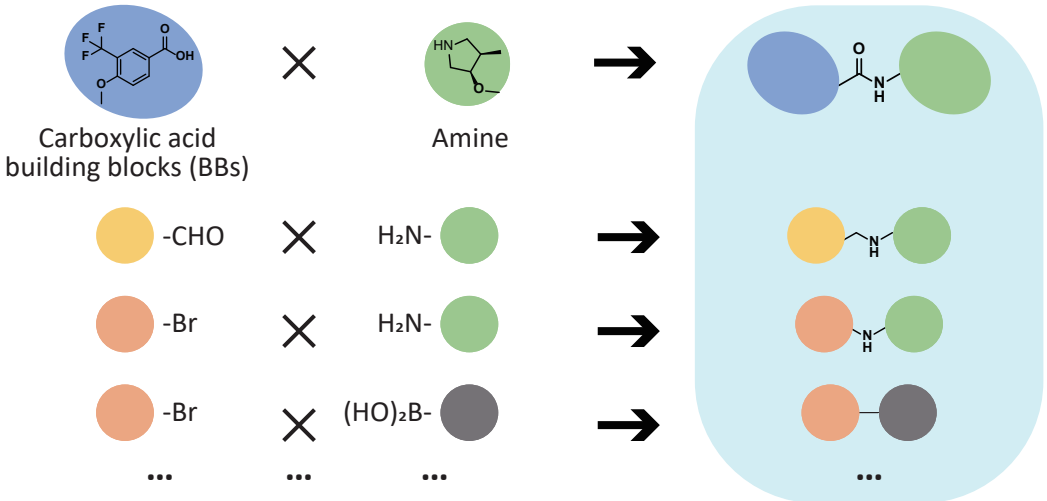
QED: Quantitative Estimate of Drug-likeness



High ratio of in-house compounds designed by medicinal chemists



Combinatorial Virtual Library (FARMING)



FARMING Library
> 10B
virtual compounds

>10B
Combinatorial virtual library

FARMING Fast-Accessible & Rapid ModifyING System

- >10B combinatorial virtual library consists of Axcelead's proprietary stock building blocks
- Semi-automated design based on structure similarity and chemical property similarity
- Utilization of high-throughput synthesis platform, the virtual compounds can be rapidly synthesized

Maximized HTS Efficiency by Computational Chemistry & AI/ML

Integrated HTS platform

- HTS strategy design
- Material preparation
- Assay development
- Pilot screening
- Primary screening
- Retest & Counter
- Dose response
- Compound purity test
- Hit report
- Hit expansion
- ADMET profiling
- Lead generation

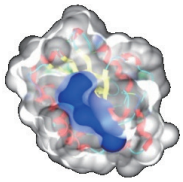
Structure based virtual screening platform

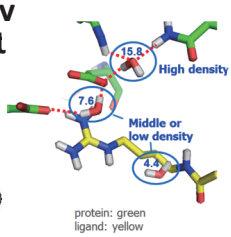
A-code

Pocket

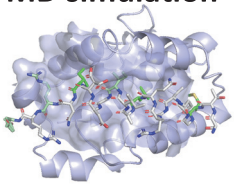
Dynamics

Ligandabilitv assessment





MD simulation

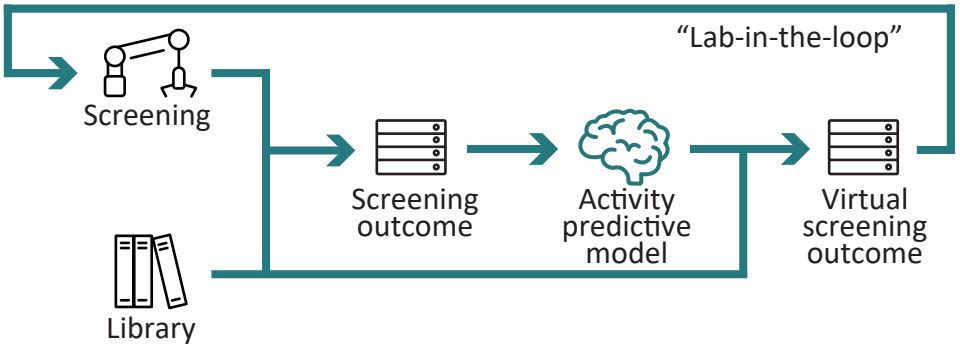


LigMap
Hot spot analysis

MMPBSA
Binding free energy calculation

- **Original annotation information based on proprietary assay database**
- **ADME prediction model for hit prioritization**

- **Structure-based similarity search from >1.2M compound library and 10B virtual library**
- **Virtual screening utilizing AI/ML model, trained by using primary HTS data**



Axcelead is a leading drug discovery CRO, established in 2017 as a spin-off from Takeda Pharmaceutical Company, inheriting the research functions, data, and human resources related to preclinical drug discovery capabilities including HTS.

Axcelead can utilize the proprietary >1.2M compound library inherited from Takeda, which can provide unique hits that cannot be obtained from commercial HTS libraries. HTS libraries are to be selected carefully for each HTS projects based on our HTS experiences over 700 projects, and we have successfully identified hit compounds in more than 90% of the recent projects. Axcelead's HTS library is divided into three types: the diversity library, the focused library, and the virtual library. The focused library is a collection of purpose-oriented libraries, including those selected based on compound properties, those targeting specific target classes, and those for RNA-targeting small molecules and molecular glue degraders, which represent the latest trends in small molecule drug discovery. The virtual library, consisting of >10B compounds, is derived form Axcelead's diverse building blocks and can be efficiently used for virtual screening and initial SAR analysis. This process is accelerated through semi-automated design systems and high-throughput synthesis, utilizing readily available stock compounds to expedite early-stage drug discovery.

Axcelead's HTS platform integrates advanced computational chemistry, AI, and machine learning to optimize screening strategies. For instance, structure-based virtual screening is performed using A-code, a proprietary set of computational chemistry tools, while AI models trained on screening data help identify additional hits from Axcelead's compound library. With comprehensive preclinical drug discovery capabilities, Axcelead provides seamless support from hit identification through the candidate selection stage. You can rely on Axcelead's unique compound library and expertise, augmented by cutting-edge technologies such as computational chemistry and AI.

Integrated HTS platform

HTS plan proposal → Assay development → HTS → High quality hit compounds → Candidate

Comprehensive experience for various target classes

Pharma-origin compound library

Computational and AI/ML approach to maximize HTS & LG efficiency

>700	>90%	>610	>480	>80%
Screening experience	Successful hit finding	Protein prep. in 6 years	Assay developments in 6 years	Assay developed at Axcelead

Comprehensive Experience in HTS and Hit Profiling

Enzyme

- Luminescence, absorbance, coupling, fluorescence, TR-FRET, AlphaScreen
- Label-free assay (Rapidfire-MS)
- ELISA
- Radiometric assay

Protein/Protein Interaction

- TR-FRET, AlphaScreen
- ELISA
- NanoBit®, NanoBRET®
- Two-hybrid assay
- Biophysical assay

Nucleic Acids (DNA, RNA)

- Biophysical assay (e.g. ASMS)
- Fluorescence probe binding
- FRET
- Cell-based assay (Reporter gene, RT-qPCR)

GPCR

- cAMP assay
- Ca2+ flux assay (FLIPR, FDSS)
- Reporter gene assay
- Arrestin/internalization assays
- Binding assay (ASMS)

Ion Channel/Transporter

- Ion influx assay
- Membrane potential
- Electrophysiology
- Substrate uptake
- Binding assay (ASMS)

Nuclear Receptor

- Cofactor recruitment assay
- Reporter gene assay
- Nuclear translocation assay

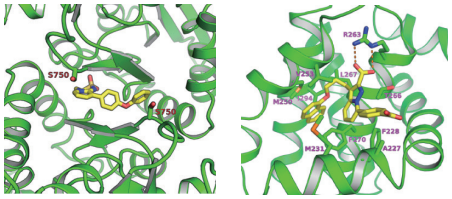
Phenotype

- High content imaging assay
- Reporter gene assay
- qRT-PCR
- Cell growth, etc.

Biophysics

- SPR, BLI
- ASMS
- ITC
- TSA

X-ray Crystallography



Axcelead Drug Discovery Partners, Inc.
https://www.axcelead-us.com/

WEB LinkedIn

SCRN_HTS001E_202409