Solution Provider for Drug Discovery

Axcelead Drug Discovery Partners, Inc.

AXCELEAD
Drug Discovery Partners

High-throughput screening (HTS)

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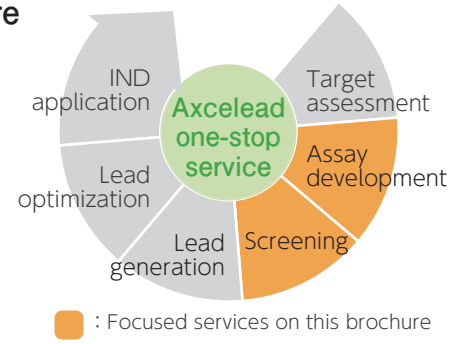
Our HTS platforms and services for your drug discovery

- Seamless services from assay development through HTS with well-experienced and high expertise professionals
- HTS platform covering a wide range of target classes and phenotypes
- Pharma-origin vast library with high quality and diverse structure
- One-stop Hit follow-up service

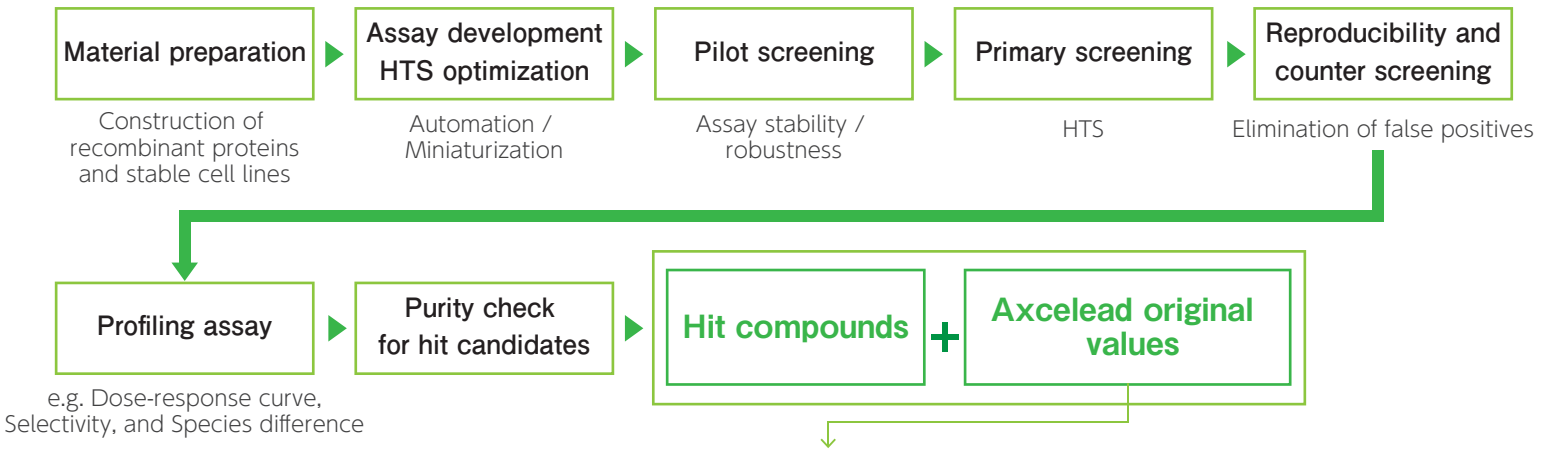
> 600 projects	> 90%	> 1.5 million
HTS experience	High success rates in hit identification	Axcelead Compound library



Seamless screening platform from assay development through HTS with well-experienced and high expertise professionals

- Axcelead offers an integrated screening platform including material preparation, assay development, and HTS.
- Axcelead proposes promising flexible screening plans and strategies based on customer needs.

■ Axcelead comprehensive screening services



- Axcelead provides hit compounds including high-value information.
  - Compound profiles based on Axcelead original data.
    - Cytotoxicity data (only for compounds tested in-house so far)
    - Biological annotations of hit compounds (only for compounds tested in-house so far)
      - Axcelead provides information on possible target classes (such as GPCR, kinase, enzyme…) that your hit compounds could modulate based on Axcelead original and public data.
    - Kinase selectivity profiles
      - Axcelead provides kinase selectivity data (> 300 kinases) for your hit compounds (only for compounds tested in-house so far).
  - Review of hit compounds by medicinal chemists in Axcelead
    - Clustering of hit compounds by Axcelead original algorithm
    - Comments on structural characteristics of each cluster
  - Drug-like properties (QED, HBA/HBD, AlogP, tPSA, number of aromatic ring, Fsp3 etc.)

<Result report image>

Compound No	Cluster ID	Primary assay (C50(nM))	Counter assay (C50(M))	Primary assay (Graph)	Counter assay (Graph)	Chemical properties				Purity (%)	Notes
						MW	HBD	HBA	AlogP		
AXL1	1	8.0E-08	>1.0E-05							95.5	kinase A inhibitor
AXL2	1	2.9E-07	>1.0E-05							90.5	kinase A inhibitor
AXL3	1	4.9E-06	>1.0E-05							95.3	kinase A inhibitor
AXL4	2	3.2E-08	>1.0E-05							85.4	promiscuous
AXL5	3	1.2E-06	>1.0E-05							97.2	
AXL6	3	2.5E-06	>1.0E-05							98.1	
AXL7	3	4.2E-06	>1.0E-05							95.4	

Assay development and high-throughput screening platforms covering a wide range of target classes

- Platforms are available for all major target classes and phenotypes.
- Axcelead proposes and conducts suitable material preparation (recombinant proteins and stable cell lines) for your HTS.

Please feel free to contact us

Major AXL assay platforms

- GPCRs
- Enzymes
- Ion channels/Transporters
- Nuclear receptors
- PPI (protein-protein interaction)
- Phenotypic screening

e.g.) High content screening, Reporter gene assay, Gene expression analysis


IN Cell Analyzer 6000 (GE Healthcare)


HORNET HTS-10CB (FUJIFILM Wako)


RapidFire MS (Agilent)


Syncropatch 384 (Nanion)

Vast compound libraries with high quality and diverse structure

- Axcelead proposes the optimal compound libraries for your HTS.

AXL compound library

1.5 million compounds

Diversity libraries

- Pooled library* **782,000** compounds
- Single library **79,000** compounds

*: The pooled library consists of samples of 10 different compounds in a single well. It enables an efficient and large scale HTS.

- You can choose either or both of pooled and single libraries that pursue lead-likeness and diversity.

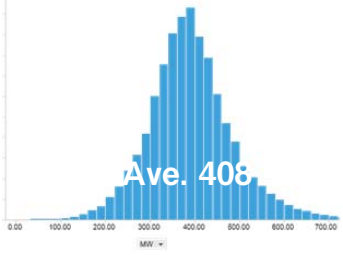
Focused libraries **100,000** compounds

- Libraries for target classes (Kinase, GPCR, Protease, PPI, etc.)
- CNS
- Covalent
- Fragment
- Macrocyclic
- Extended rule of 5
- Natural product
- sp^3 rich
- Phenotypic-oriented
- Annotation

- Low cytotoxic compounds and annotation libraries for phenotypic screening are also available.

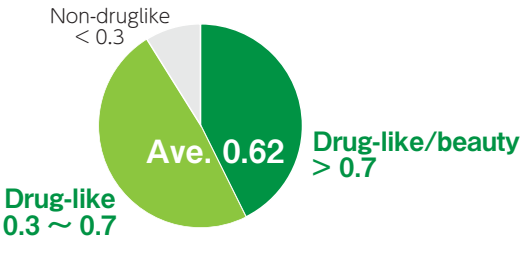
High quality compound library

Diversity of molecular weight distribution

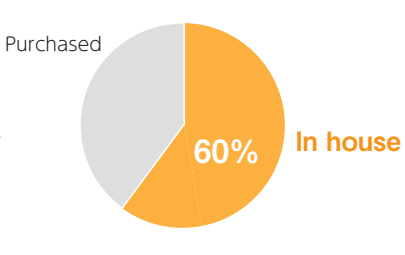


High drug-likeness

QED: Quantitative Estimate of Drug-likeness



High ratio of in-house compounds designed by medicinal chemists



For customers who have received our HTS service

One-stop Hit follow-up service after HTS

▶ **Axcelead supports to generate Advanced Hit compounds with several approaches to prioritize your hit chemotypes.**

HTS

Hit compounds

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Hit follow-up service

- Prioritization of the Hit chemotypes -

Exploration of initial SARs

・Additional screening of Axcelead library compounds
・Building a small compound library using high-throughput parallel synthesis

In vitro activity evaluation

・Biochemical and biophysical analysis

ADMET profiling

・CYP inhibition, PAMPA, Solubility, Cytotoxicity, hERG channel inhibition, etc.

- Similarity search of hit compounds from Axcelead compound library (ca. 1.5million) and evaluation are available.
- Well-experienced Axcelead chemists in drug discovery support compound selection.
- High-throughput parallel synthesis technology provides rapid and efficient delivery of hit related derivatives.
- Axcelead provides appropriate in vitro assay systems according to your targets and evaluates the related derivatives.
- X-ray crystal structural analysis is also available.
- Axcelead offers high-throughput ADMET profiling services with extensive experience and sophisticated protocols.

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Advanced Hit

■ Axcelead biophysical analysis

- Affinity selection-mass spectrometry (AS-MS)
- Thermal shift assay (TSA)
- Nuclear Magnetic Resonance (NMR)
- Isothermal titration calorimetry (ITC)
- Surface plasmon resonance (SPR)
- X-ray crystallography

Application examples) SBDD, FBDD, MOA analysis, etc.

Triple. Quadrupole LCMS (Agilent)

Biacore S200 (GE Healthcare)

MicroCal iTC200 (Malvern Panalytical)

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