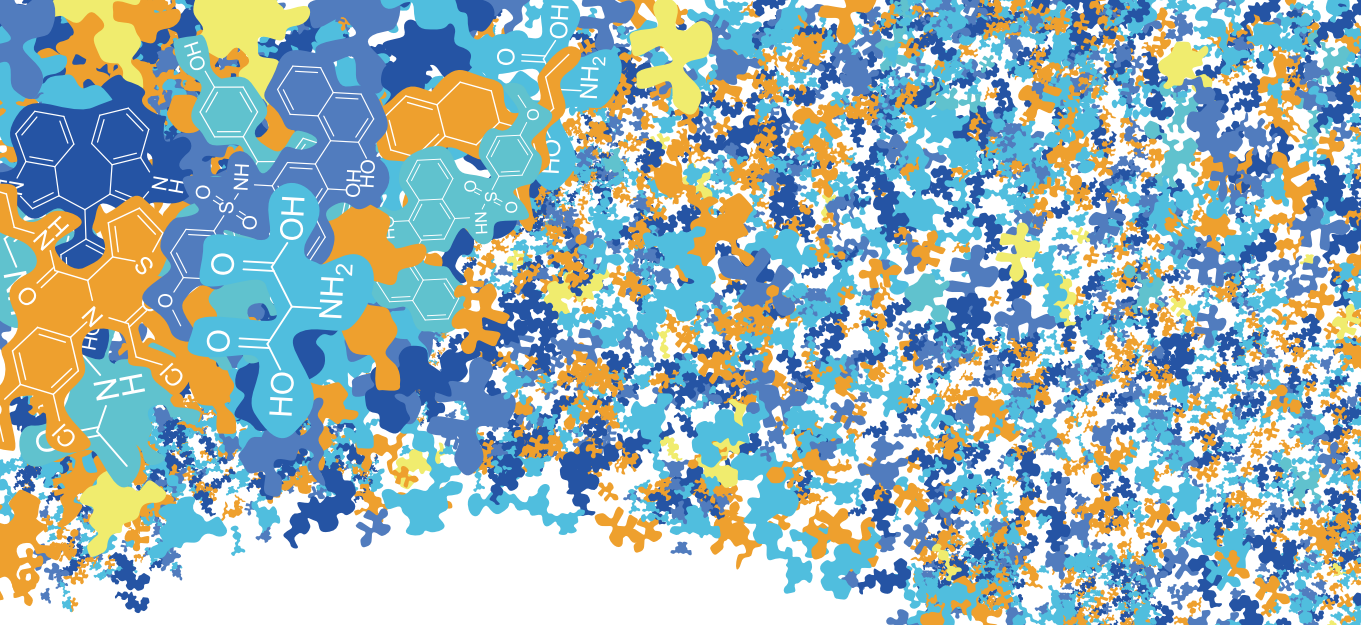
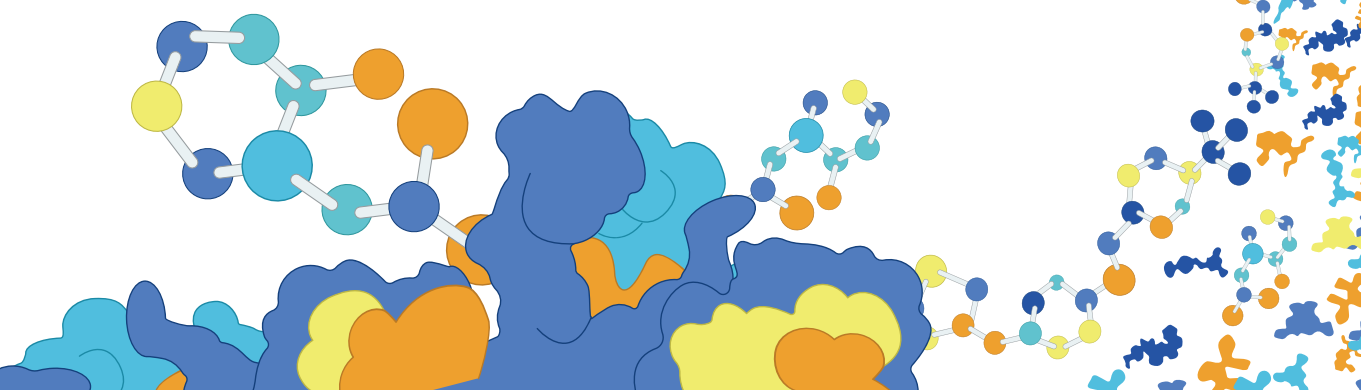


German distributor:

Hycultec GmbH
Tel.: 08543/916182
info@hycultec.de
www.hycultec.de

Compound Screening Libraries

Accelerating Early Drug Discovery



Drug Discovery

Drug discovery and development is a time-consuming and high-cost process; including early drug discovery, pre-clinical studies, clinical development, FDA review, and post-market monitoring. Early drug discovery is a key step in drug discovery and development process. Nowadays, early drug discovery involves target identification & validation, screening hits, and optimization of hits, etc. With the development of chemical synthesis and natural products extraction technology, large numbers of small molecule compounds are available for screening. High throughput screening (HTS) technology accelerated the hit discovery process. In recent decades, approaches such as fragment-based drug discovery (FBDD), structure-based drug discovery (SBDD), drug repurposing and repositioning, and virtual screening, have been exploited to reduce the cost and increase the success rate of drug discovery and development.

Basic Research	Preclinical Development	Clinical Trials	FDA Filing/Approval

MCE Compound Library

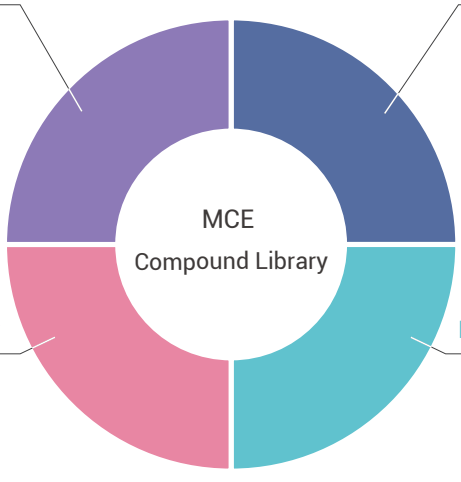
- HTS compound database, molecular docking and virtual screening service
- **30,000+** bioactive compounds with clear target and function annotation
- **18,000+** fragment compounds with diverse structures
- Customized libraries are also available

Fragment Library

- **18,000+** fragment compounds
- Diverse structure
- Useful tool for **fragment-based drug discovery** (**FBDD**)

Bioactive Compound Library

- **100+** bioactive compound libraries
- **30,000+** bioactive compounds are supplied
- Covering **500+** targets and hot research areas



Customized Compound Library

- Specific Compounds
- Plate Map
- Size
- Form (Solid or DMSO Solution) …

High Throughput Screening Library

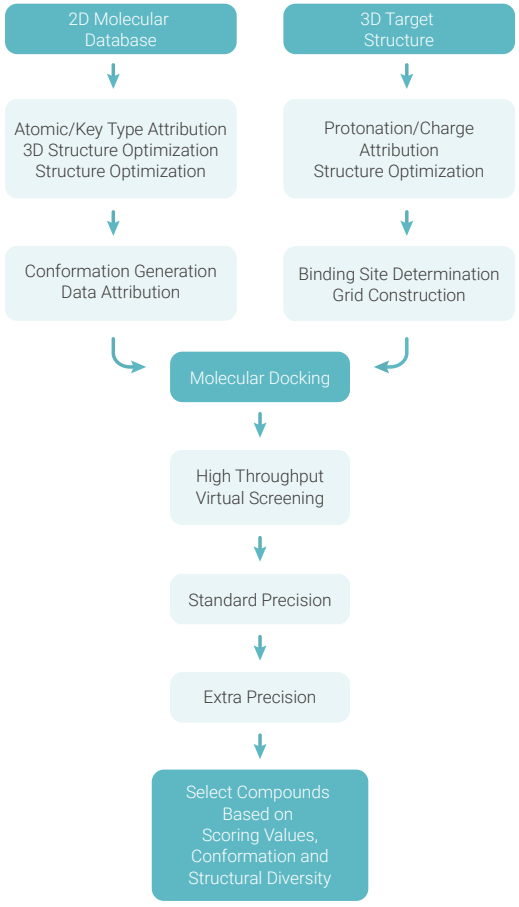
- **16 million** compounds are available
- Diverse structure and Drug-like feactures
- All compounds are in stock and can be resupplied

MCE Virtual Screening

Virtual screening is a computational technique that automatically searches large libraries of small molecules in order to identify those structures which most likely to bind to a drug target. It has become an integral part of the early drug discovery process.

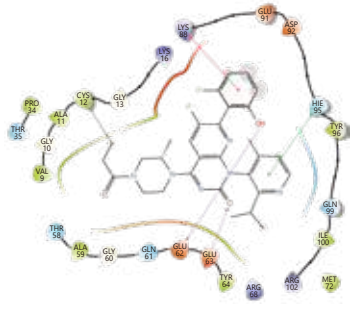
MedChemExpress (MCE) provides high quality virtual screening service that enables researchers to efficiently identify scaffolds with promising structure activity relationship (SAR). Our optimized virtual screening protocol can reduce the size of chemical library to be screened experimentally, increase the likelihood to find innovative hits in a faster and less expensive manner, and mitigate the risk of failure in the lead optimization process.

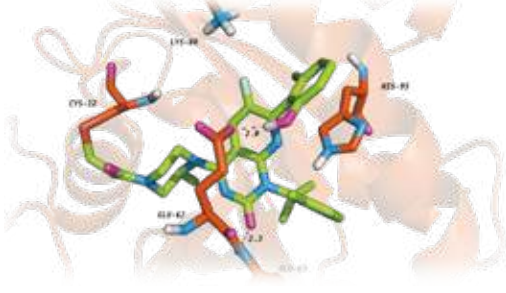
MCE offers versatile HTS compound databases covering 16 million in-stock, reproducible, structurally diverse, drug-like compounds. MCE's virtual screening service truly realizes ultra-high-throughput compound library + cloud computing platform = unlimited possibilities.



A classic case:

The structure model diagram of Sotorasib binding KARS G12C: The acrylamide double bond of Sotorasib covalently binds to the amino acid residue Cys12 of KARS G12C. The carboxyl group on the benzene ring of Sotorasib acts as a hydrogen bond donor to form a hydrogen bond with residue Glu62, and the hydrogen bond distance is 2.3 Å. In addition, the compound not only forms a π-π stacking interaction with the residue His95, but 2-fluoro-6-hydroxyphenyl can also form a cation-π interaction with the residue Lys88.



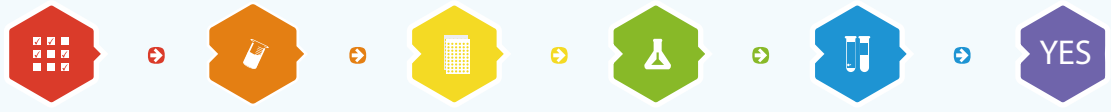


MCE Bioactive Screening Libraries

Our ready-to-use MedChemExpress (MCE) compound libraries consist of over **30,000** small molecules with validated biological and pharmacological activities. They are available for **high-throughput screening (HTS)** and **high-content screening (HCS).** Bioactive compound libraries are useful tools for drug repurposing and new indication research.

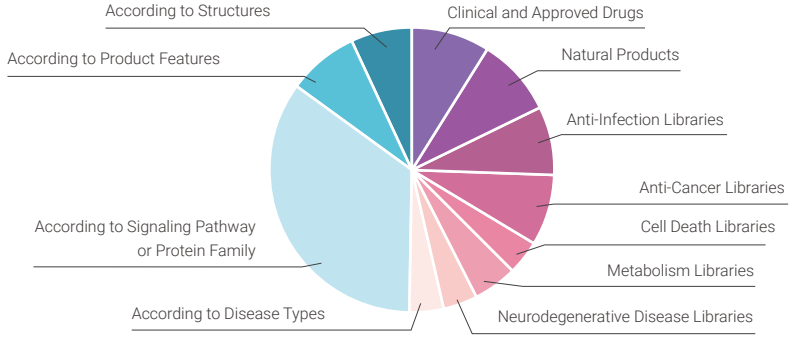
- Safety and effectiveness have been confirmed by literatures, patent reports and clinical researches.
- Focuses on hundreds of targets that are key components in the fields of **GPCRs, kinases, cancer, epigenetics and stem cell biology,** etc.
- Libraries are updated every week by adding newly published small molecules in the related fields, providing customers with a more comprehensive and innovative choice.
- MCE provides detailed biological and chemical information on every compound together with the **LC/MS** and **NMR** reports to ensure high quality.
- MCE offers customized compound libraries based on your specific needs. You can select the compounds' format (powder/liquid), size and plate map depending on your requirements.

Customize Your Library



Specific Compounds → Quantities → Plate Map → Concentration → Form (Solid or Solution) → YES

According to the signaling pathways, research areas, clinical data and other features of products, compound libraries can be classified into several types, such as FDA-approved drug library, kinase inhibitor library, etc. We can now supply more than 100 types of compound libraries, including drug repurposing libraries, natural products, anti-microbial compounds libraries, cancer related libaries, and cell death related libraries.



Our Advantages

Complete Product Categories and Quick Updates

30,000 + bioactive compounds, 16 million screening compounds and 16,000 + fragment compounds can be selected based on your specific needs. New compounds are launched and added to our libraries regularly to ensure their comprehensiveness.

Perfect Product and Data Management System

Our compound library preparation is automated and all products can be traced to avoid human error. Each product is supplied with detailed bioactivity information and physicochemical properties.

Rigorous Classification Criteria

Based on a large number of literatures and authoritative database analysis, we set accurate classification standards for each library.

Strict Quality Management System

Certified by ISO 9001 quality management system, with state-of-the-art R&D and manufacturing facilities, strict quality control and verification system.

Professional Service

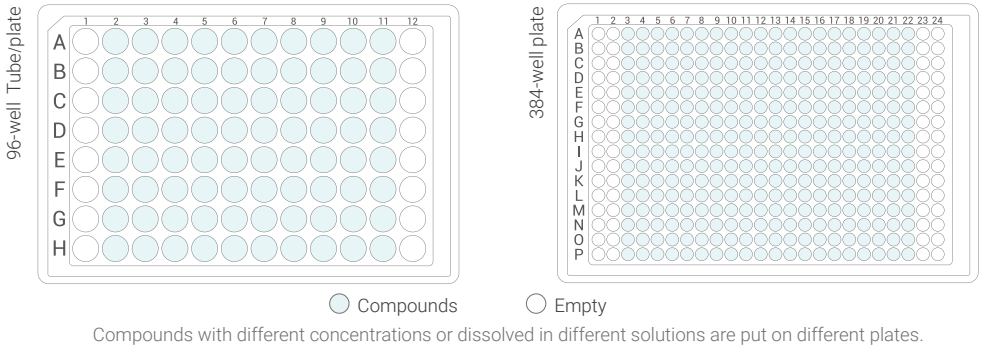
MCE can provide you with the professional technical support along with the high-quality products at the most competitive price and the shortest delivery time.

Customize Library

You can select

- √ Specific Compounds
- √ Quantities
- √ Plate Map
- √ Concentration
- √ Form (Solid or Solution)

Bioactive Compound Library Parameters

	96-well Format Sample Storage Tube	96-/384- well plate
		
Specifications	30 μL, 50 μL, 100 μL or other size lower than 750 μL	96-well plate: 30 μL, 50 μL, 100 μL or other size lower than 100 μL 384-well plate: 30 μL, 50 μL or other size lower than 50 μL
Sealing Way	Screw Cap	Peelable Foil Seal
Concentration	**10 mM** solution for products with stable solution state and solubility no less than 10 mM; **2 mM** solution for products with solubility between 2 mM and 10 mM; **3 mg/mL** solution for products with unconfirmed molecular weight and solubility no less than 3 mg/mL.	
Solvent	DMSO, Water, Ethanol.	
Recommended Storage Time	-20°C for 1 year; -80°C for 2 years	
Information Shipped with Library	**Product information** including targets, bioactivity information, research areas, clinical data, etc.; **Product layout** for each plate; **SDF file**, contains structure information and requires some specialized software to open (ChemOffice).	
Plate Layout	 Compounds with different concentrations or dissolved in different solutions are put on different plates. If you have any other requirements for the compounds layout, please let us know before you make the order.	

Publications Citing Use of MCE Products:

Nature. 2022 May;605(7910):567-574.
Nature. 2022 Jun;606(7915):776-784.
Nature. 2022 May;605(7911):747-753.
Nature. 2022 May;605(7909):325-331.
Nature. 2022 Apr;604(7906):541-545.
Nature. 2022 Apr;604(7904):160-166.
Nature. 2022 Apr;604(7904):134-140.
Nature. 2022 Mar;603(7901):477-481.
Nature. 2022 Mar;603(7899):159-165.
Nature. 2022 Mar;603(7899):138-144.
Science. 2022 Mar 18;375(6586):1254-1261.
Science. 2021 Nov 26;374(6571):1099-1106.
Science. 2021 Oct;374(6563):eabf3067.
Science. 2021 Jul 30;373(6554):547-555.
Science. 2021 Apr 30;372(6541):eaba8490.
Science. 2021 Mar 5;371(6533):eabb2224.
Cell. 2022 Jun 9;S0092-8674(22)00651-1.
Cell. 2022 May 11;S0092-8674(22)00526-8.
Cell. 2022 Apr 28;185(9):1521-1538.e18.
Cell. 2022 Jan 6;185(1):158-168.e11.
Cell. 2021 Oct 28;184(22):5670-5685.e23.
Cell. 2021 Oct 14;184(21):5375-5390.e16.
Cell. 2021 Sep 16;184(19):4919-4938.e22.
Cell. 2021 Sep 2;184(18):4753-4771.e27.
Cell. 2021 Aug 19;184(17):4579-4592.e24.
Cell. 2021 Jun 10;184(12):3143-3162.e32.
Cell. 2021 Jun 24;184(13):3528-3541.e12.
Cell. 2021 Apr 15;184(8):2167-2182.e22.
Cell. 2021 Apr 1;184(7):1693-1705.e17.

Table of Contents

Cat. No.: HY-L001, HY-L001P

Bioactive Compound Library

(96-/384-well plate)

Cat. No.	Product Name	Compound Number	Supply Form
HY-L001	Bioactive Compound Library	13,000+	Part A: Solution or Solid
HY-L001P	Bioactive Compound Library Plus	15,000+	Part A, Part B & Part C Part B: Only solid Part C: Only solid

Part B-low solubility or less stable solution: For the compounds with less solution stability and due to the short shelf life of the solution, powder packaging is recommended and can be dissolved at the time of use. For the products with low solubility, MCE also provides them in powder form.

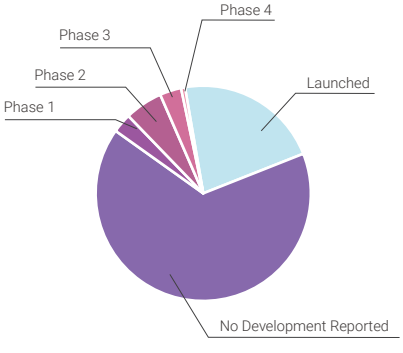
Part C-novel, rare or exclusive compounds: The products in Part C are some novel, rare or exclusive compounds, which are of high prices. MCE lists them separately and provides at least 1 mg powder packaging or ≥250 μL solution packaging. You can also choose based on your specific needs.

Publications Citing Use of MCE Bioactive Library Compounds

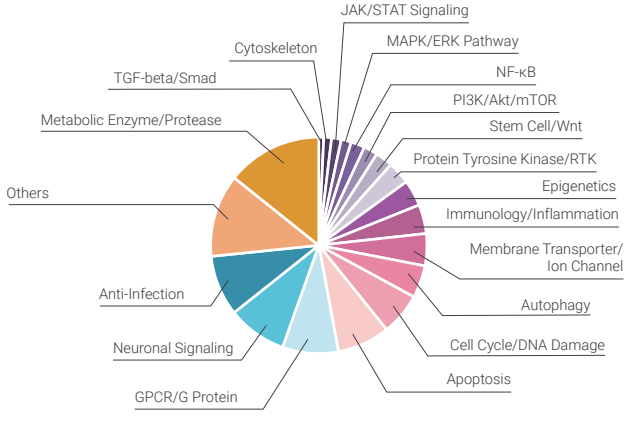
Nat Metab.2021 May;3(5):682-700. **EMBO Mol Med.** 2021 Dec 20;e14608. **Nat Commun.** 2020 Sep 4;11(1):4417. ···

Product Features

- A unique collection of **10,000+** small molecules with validated biological and pharmacological activities.
- Cover more than **500** kinds of targets, involving more than **20** major signaling pathways and several hot research areas.
- Products contain natural products, innovative compounds, approved compounds, and clinical compounds, etc. Used for signaling pathway research, drug discovery and drug repurposing, etc.
- High purity and quality validated by NMR and LC/MS.



Clinical phase for bioactive compounds

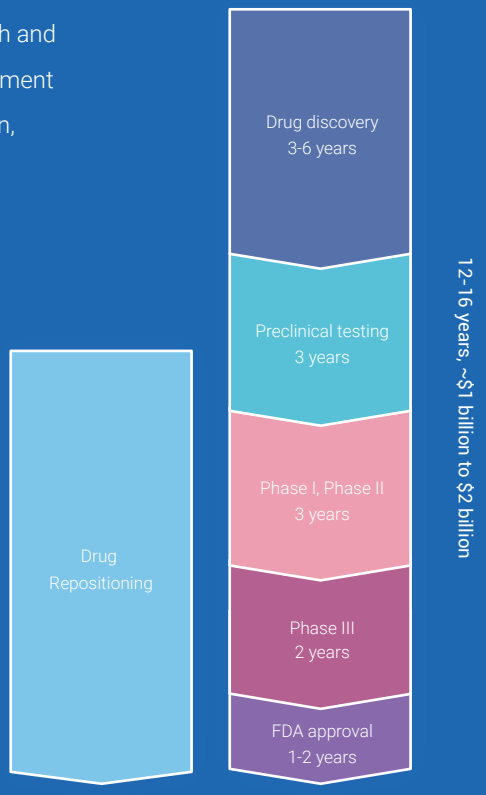


Signaling pathways of bioactive compounds

Drug Repurposing Series

Drug repurposing is a new trend in drug development. Compared with new drug development, drug repurposing has the following advantages:

Drug safety has been widely verified at the clinical stage and in the pharmaceutical market, which reduces the risk of drug development failure caused by safety. The drugs have gone through systematic pre-clinical and clinical studies, with comprehensive research and complete data. Thus, they can greatly shorten the research and development cycle. Compared with development of new drugs for the same indication, drug repurposing can greatly save research costs.



Advantage comparison between drug repurposing and development of new drugs.

Getting a drug to market currently takes 12–16 years and between US$1 billion and $2 billion on average, and the costs are going up. But some estimates suggest that repositioning drug costs on average $300 million and takes around 6.5 years. [1]

Reference: [1] Nature. 2016 Jun 16;534(7607):314-6.

Cat. No.: HY-L022, HY-L022P & HY-L022M

FDA-Approved Drug Library

(96-/384-well plate)

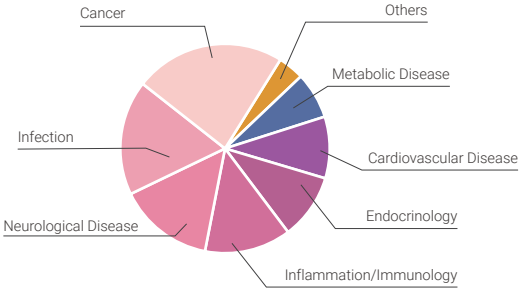
Cat. No.	Product Name	Compound Number	Supply Form	Package	Features
HY-L022	FDA-Approved Library	2,400+	Part A: Solution or powder	96-well storage tubes; 96-well/384-well microplate	High cost performance
HY-L022P	FDA-Approved Library Plus	2,600+	Part A & Part B Part B: Powder only	96-well storage tubes; 96-well/384-well microplate	A more powerful screening capability
HY-L022M	FDA-Approved Library Min	1,900+	Solution only (10 μL/well)	96-well microplate	Low price, fast delivery

Publications Citing Use of MCE FDA-Approved Library Products

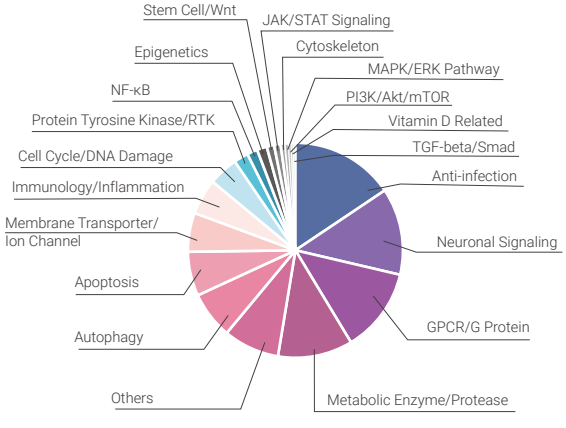
Nat Commun. 2021 Jan 12;12(1):280. **Sci Adv.** 2021 Dec 24;7(52):eabb3673. **Pharmacol Ther.** 2021 Jun 23;228:107930. ···

Product Features

- All compounds have been approved by **FDA, EMA, NMPA** and other countries. Approved agencies for every drug are available. Nearly **70%** of the drugs in this library are FDA-approved.
- Rigorous classification criteria: MCE FDA-Approved Drug Library does not contain veterinary drugs, Inactive Ingredients, food additives or compounds that are included in NDC or DMF but have not been approved for drugs.
- Cover more than 200 common targets and a variety of hot research areas, such as **oncology, infection, immunity, cardiovascular disease** and **nervous system diseases**.
- **FDA-Approved Drug Library Plus (HY-L022P)** further complements **FDA-Approved Drug Library (HY-L022)** by adding some compounds with low solubility or less solution stability and some novel, rare or exclusive compounds (Part B) to this library. All those supplementary are supplied in powder form.



Research areas involved in the FDA-approved drug library



Signaling pathways involved in the FDA-approved drug library

Cat. No.: HY-L066

FDA Approved & Pharmacopeial Drug Library

(96-/384-well plate)

Product Features

- **3,000+** compounds. Besides the approved drugs, the compounds from pharmacopoeia, **NDC** or **DMF** are also included in **FDA Approved & Pharmacopeial Drug Library.** These compounds have identified safety compared with those which have not entered any clinical studies.
- Further expands the screening capacity of the FDA-Approved Drug Library and provides a wider screening range for the drug repurposing.
- Approval agency and pharmacopoeial source for each compound are available.
- Covers a more comprehensive range of targets and research areas.

Examples of Targets included in This Library

≥100 29-99 0-28

- 5-Alpha Reductase
- Adrenergic Receptor
- ACE
- Autophagy
- Carbonic Anhydrase
- COX
- DNA/RNA Synthesis
- Estrogen Receptor/ERR
- FGFR
- HCV
- Histone Methyltransferase
- Integrin
- Microtubule/Tubulin
- P2Y Receptor
- Phosphatase
- Progesterone Receptor
- ROCK
- 5-HT Receptor
- Akt
- Antibiotic
- Bacterial
- Chloride Channel
- CXCR
- Drug Metabolite
- Factor Xa
- Fungal
- HDAC
- HIV
- Interleukin Related
- MMP
- Parasite
- Phosphodiesterase (PDE)
- Proton Pump
- SGLT
- AChE
- Aldose Reductase
- Antifolate
- Btk
- Cholecystokinin Receptor
- Cytochrome P450
- EGFR
- Farnesyl Transferase
- Gap Junction Protein
- HIF/ HIF Prolyl-Hydroxylase
- iGluR
- LPL Receptor
- nAChR
- PARP
- PKC
- Reactive Oxygen Species
- Topoisomerase
- Adenosine Receptor
- Angiotensin Receptor
- Apoptosis
- Calcium Channel
- c-Kit
- DHODH
- Endogenous Metabolite
- Ferroptosis
- GSK-3
- Histamine Receptor
- Influenza Virus
- mAChR
- NKCC
- PDGFR
- Potassium Channel
- RET
- VEGFR

Publications Citing Use of MCE FDA Approved & Pharmacopeial Library Products

Cancer Lett. 2020 Apr 28;476:67-74.
Cell Death Dis. 2019 Aug 13;10(8):615.
Nat Med. 2019 Sep;25(9):1428-1441.
Cancer Lett. 2020 Apr 28;476:67-74.
J Exp Clin Cancer Res. 2021 Sep 22;40(1):297.
Acta Pharmacol Sin. 2021 Jan;42(1):108-114.

Cat. No.: HY-L053

NMPA-Approved Drug Library

(96-/384-well plate)

Product Features

- A unique collection of **1,200+** NMPA-approved compounds that could be used for HTS and HCS.
- All the compounds have undergone extensive preclinical and clinical trials, showing good bioactivity, safety and bioavailability.
- A useful tool for drug repurposing which could dramatically accelerate drug development.
- More detailed compound information with structure, IC_{50}, and brief introduction.
- High purity and quality validated by NMR and LC/MS.

Cat. No.: HY-L026 & HY-L026P

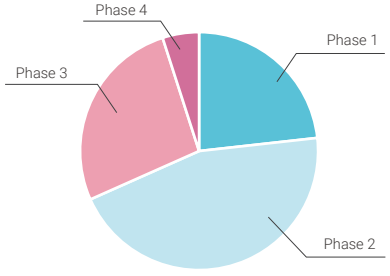
Clinical Compound Library

(96-/384-well plate)

Cat. No.	Product Name	Compound Number	Supply Form
HY-L026	Clinical Compound Library	1,700+	Part A: Solution or powder
HY-L026P	Clinical Compound Library Plus	1,900+	Part A & Part B Part B: Powder only

Product Features

- All compounds were reported in the authoritative clinical database. Clinical information for each compound is available.
- Compounds in this library include clinical compounds and drugs withdrawn from the market (Phase IV).
- Cover **260+** commonly used targets and a variety of hot research areas, such as cancer, immunity, infection, cardiovascular, etc.
- **HY-L026P,** with a more powerful screening capability, further supplements **HY-L026** by adding some compounds with low stability or low solubility and some novel, rare or exclusive compounds (Part B). Supplementary compounds are provided in powder form.



Clinical phases of clinical compound library

Cat. No.: HY-L035 & HY-L035P

Drug Repurposing Compound Library

(96-/384-well plate)

Cat. No.	Product Name	Compound Number	Supply Form
HY-L035	Drug Repurposing Compound Library	3,800+	Part A: Solution or powder
HY-L035P	Drug Repurposing Compound Library Plus	4,100+	Part A & Part B Part B: Powder only

Product Features

- Compounds include **approved drugs** and **clinical drugs passing phase I**.
- Compounds in this library have identified bioactivities, good pharmacokinetic characteristics and safety, which are suitable for drug repurposing.
- Detailed bioactivity information including target, clinical data, etc. is available.
- Cover more than **300** kinds of commonly used targets, involving a variety of hot research areas.
- **HY-L035P**, with a more powerful screening capability, further supplements **HY-L035** by adding some compounds with low stability or low solubility and some novel, rare or exclusive compounds (Part B). Supplementary compounds are provided in powder form.

Examples of Targets in these Libraries

● ≥ 60 ● 20-59 ● 0-19

- 5-Alpha Reductase
- Adenosine Receptor
- AMPK
- ACE
- Btk
- CGRP Receptor
- COMT
- DNA/RNA Synthesis
- Endogenous Metabolite
- Factor Xa
- HCV
- mAChR
- Opioid Receptor
- Serotonin Transporter
- 5-HT Receptor
- Akt
- Amyloid-β
- Aromatase
- Calcium Channel
- Chloride Channel
- COX
- Dopamine Receptor
- Endothelin Receptor
- iGluR
- Microtubule/Tubulin
- Phosphodiesterase (PDE)
- SGLT
- AChE
- Aldose Reductase
- Androgen Receptor
- Bcl-2 Family
- CaSR
- Cholecystokinin Receptor
- CRISPR/Cas9
- EGFR
- Epoxide Hydrolase
- GABA Receptor
- JAK
- Monoamine Oxidase
- Potassium Channel
- Sodium Channel
- ADC Cytotoxin
- ALK
- Angiotensin Receptor
- Bradykinin Receptor
- CDK
- c-Kit
- Cytochrome P450
- Elastase
- Estrogen Receptor/ERR
- Glucocorticoid Receptor
- LPL Receptor
- Neurokinin Receptor
- Progesterone Receptor
- Thyroid Hormone Receptor

Natural Products Series

The structural diversity of natural products and their easy binding with biomacromolecules determine their incomparable advantages in the process of life regulation and endue natural products with an irreplaceable important position in the research and development of new drugs. Natural products and their molecular frameworks are the main sources of new drugs, in fact, about two-thirds of all drugs approved between 1981 and 2019 are, at different extents, related to natural products [1].

MCE can provide natural products and natural product analogues from a variety of sources, including plants, animals, and microorganisms. The compounds in the library contain Saccharides & Glycosides, Phenylpropanoids, Quinones, Flavonoids, Terpenoids and Glycosides, Steroids, Alkaloids, Phenols, Acids and Aldehydes.

MCE natural products have clear source information and structure classification for data analysis. Natural products and analogues available from MCE are as follows:

Reference: [1] J Nat Prod. 2020 Mar 27;83(3):770-803.

Cat. No.: HY-L021 & HY-L021P

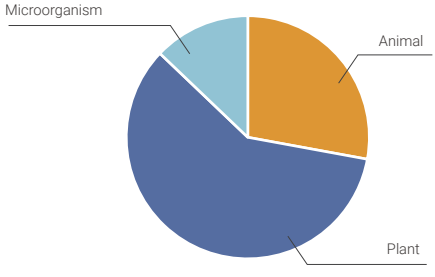
Natural Product Library

(96-/384-well plate)

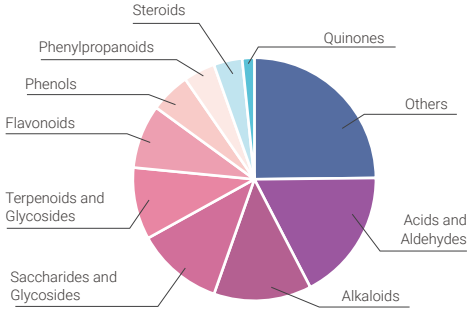
Cat. No.	Product Name	Compound Number	Supply Form
HY-L021	Natural Product Library	3,200+	Part A: Solution or powder
HY-L021P	Natural Product Library Plus	3,600+	Part A & Part B Part B: Powder only

Product Features

- All natural products have clear sources and structure classifications.
- Structurally diverse, including **Saccharides** and **Glycosides, Phenylpropanoids, Quinones**, **Flavonoids, Terpenoids** and **Glycosides, Steroids, Alkaloid, Phenols, Acids** and **Aldehydes,** etc.
- Bioactivity and safety have been confirmed by clinical trials and/or preclinical research. Some compounds have been approved by FDA.
- Bioactivity diversity, covering 200+ common targets, 20+ hot signaling pathways and a variety of research areas.
- **HY-L021P,** with a more powerful screening capability, further supplements **HY-L021** by adding some compounds with low solution stability or low solubility and some novel, rare or exclusive compounds (Part B). Supplementary compounds are provided in powder form.



Source of products in MCE Natural Product Library



Different structure types in MCE Natural Product Library

Publications Citing Use of MCE Natural Product Library Compounds

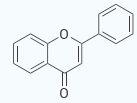
Cancer Cell. 2021 Mar 8;39(3):380-393.e8.
Cancer Lett. 2020 Jul 1;481:15-23.
Free Radic Biol Med. 2021 Dec;177:313-325.
Autophagy. 2021 Jun;17(6):1519-1542.
Sci Adv. 2021 Mar 5;7(10):eabe7853.
Clin Transl Med. 2020 Oct;10(6):e208.
Cell Biosci. 2021 Feb 28;11(1):45.
Theranostics. 2021 Apr 19;11(13):6355-6369.
Oncogene. 2020 Feb;39(7):1557-1571.

Cat. No.: HY-L056, HY-L071, HY-L068 & HY-L057

Terpenoids, Alkaloids, Flavonoids and Phenols Product Libraries (96-/384-well plate)

Product Features

- Structurally diverse, bioactive, and cell permeable.
- Bioactivity and safety have been confirmed by clinical and/or preclinical trials. Some compounds have been approved by FDA.
- More detailed compound information with structure, target, and brief introduction.
- High purity and quality validated by NMR and LC/MS.

Product Name	Induction	Product Features	Representative Structure
HY-L056 Terpenoids Library	Terpenoids display a wide array of important pharmacological properties in the fight against **cancer, malaria, inflammation**, and a variety of **infectious diseases**.	A unique collection of **400+** natural terpenoid compounds, such as **monoterpenes, sesquiterpenes, diterpenes, ester terpenes** and **triterpenes**, etc.	
HY-L071 Alkaloids Library	Alkaloids are a large and complex group of cyclic compounds that contain N. Important alkaloids include morphine, strychnine, atropine, colchicine, ephedrine, quinine, and nicotine. They show **anti-inflammatory, anticancer, analgesics, local anesthetic** and **neuropharmacological** activities, etc.	A unique collection of **500+** natural alkaloids, such as **indoles, quinolines, isoquinolines, pyrrolidines, pyridines, pyrrolizidines, tropanes,** and **terpenoids** and **steroids**.	
HY-L068 Flavonoids Library	Flavonoids have **anti-oxidative, anti-mutagenic, anti-inflammatory,** and **anti-carcinogenic** properties coupled with capacity to modulate **key cellular enzyme function**. They have been widely used in a variety of nutrition, medicine and cosmetics.	A unique collection of **350+** natural flavonoid compounds, such as **flavones, flavonols, flavanones, flavanonols, flavanols,** etc.	
HY-L057 Phenols Library	Phenolic compounds are a diverse group of naturally occurring compounds with multiple activities, such as **antioxidant** and **antimicrobial** properties.	A unique collection of **800+** natural phenol compounds with a variety of biological activities.	

Cat. No.: HY-L021L

Natural Product Like Compound Library

(96-/384-well plate)

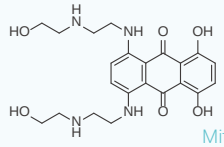
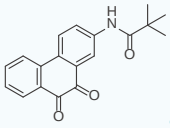
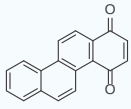
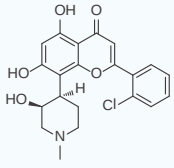
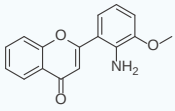
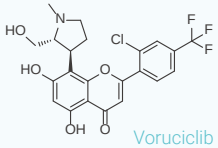
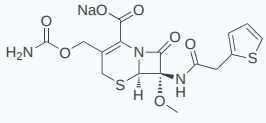
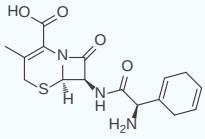
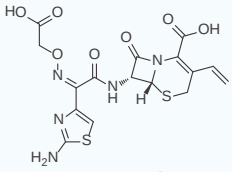
Natural products (NPs) and their molecular frameworks are the main sources of new drugs and play highly significant roles in the drug discovery and development process. Based on the source and structure analysis of 1,562 drugs approved by the FDA from 1981 to 2014, it was found that 21% of the drugs were natural product derivatives, and 61% of the drugs contained natural product pharmacophore groups. From this point, it concludes that natural product analogues and derivatives have the same screening value as natural products in the development of new drugs.

MCE provides a unique collection of **200+** natural product-like compounds that are structurally like Steroids, Tannins, Flavonoids, Isoquinolines, etc. This library is an important source of lead compounds for HTS and HCS.

Product Features

- All products are natural product analogues or derivatives and can be used in the development of new drugs.
- Structurally diverse, bioactive, and cell permeable.
- Detailed bioactivity information, including target, research areas and clinical information.
- High purity and quality validated by NMR and LC/MS.

Examples of Products in the Library

Quinones	HY-13502  Mitoxantrone	HY-15842  SF1670	HY-111441  1,4-Chrysenequinone
Flavonoids	HY-10005  Flavopiridol	HY-12028  PD98059	HY-12422  Voruciclib
Cephalosporins	HY-B1117  Cefoxitin sodium	HY-B1156  Cephradine	HY-B1381  Cefixime

Cat. No.: HY-L065

Traditional Chinese Medicine Monomer Library

(96-/384-well plate)

Traditional Chinese Medicine (TCM) has been used for centuries in China, where herbs are considered fundamental therapy for many acute and chronic conditions. Many studies indicated TCM exerted an overall regulatory effect via multi-component and multi-target network. Traditional Chinese medicine monomers are active compounds of Chinese Herbal Medicines. They possess medicinal properties such as **anti-cancer, anti-bacterial** effects may be an important source of new drugs. For example, **Artemisinin**, used in multidrug resistant malaria, was first isolated from the Chinese herb *Artemisia annua L.*

MCE designs a unique collection of **1,700+** compounds that all come from Chinese Herbal Medicines. MCE Traditional Chinese Medicine Monomer Library is a useful tool for discovering new drugs from TCM.

Product Features

- Structurally diverse, containing **Saccharides** & **Glycosides, Terpenoids** & **Glycosides, Alkaloid, Phenols, Acids** and **Aldehydes**, etc.
- Sources diverse, including ginseng, coptis, notoginseng, angelica and other 500+ Chinese herbal medicines.
- Clear source of traditional Chinese medicine and detailed bioactivity information is available.
- Bioactivity diverse, covering several hot research areas such as **immune inflammation, cancer, anti-infection, cardiovascular disease**, etc.

Cat. No.: HY-L055

Medicine Food Homology Compound Library

(96-/384-well plate)

Food as medicines have many benefits because of their safety. In order to ensure the safe use of functional food, National Health Commission of the People's Republic of China made specific provisions on Medicine Food Homology (MFH) items. More than 100 kinds of widely used MFH materials have been released.

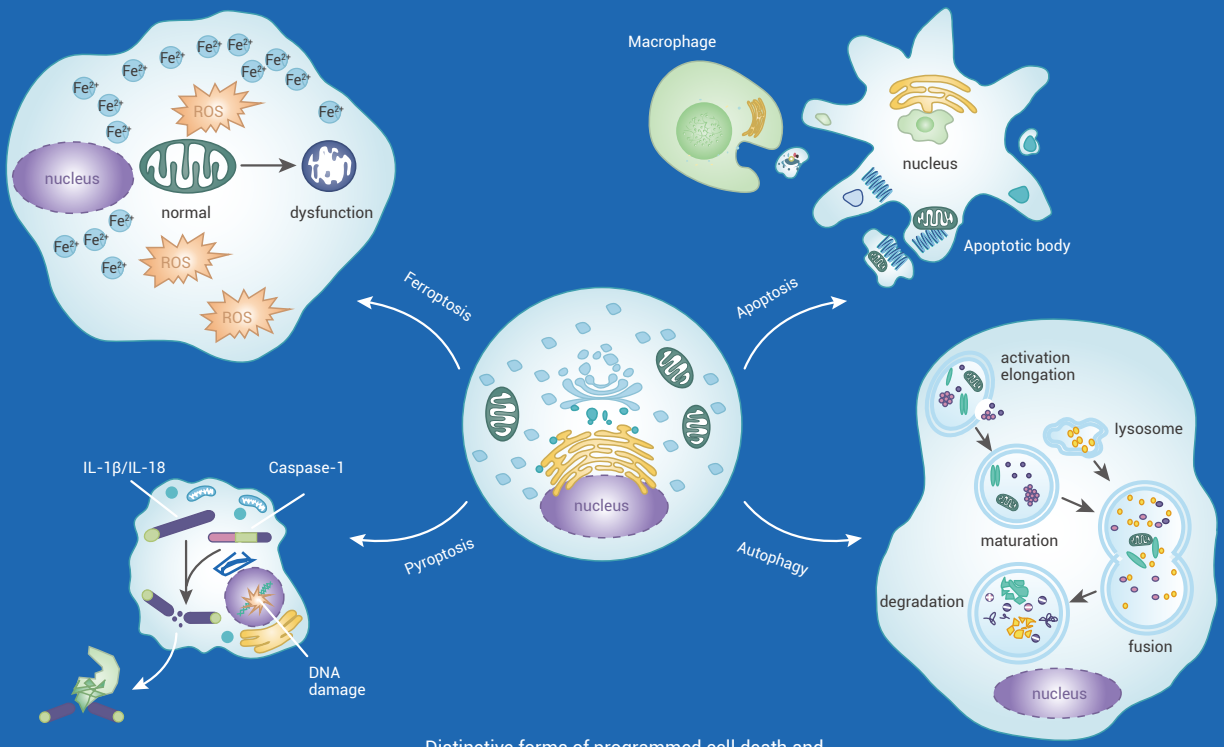
Based on MFH items released by National Health Commission, PRC, MCE carefully designs a unique collection of **600+** Medicine Food Homology Compounds with high safety.

Product Features

- All compounds are from Medicine Food Homology materials, which have high medicinal value and safety, and can be used for HTS and HCS.
- Sources diverse, those compounds are from more than 100 kinds of Medicine Food Homology materials.
- Detailed bioactivity information, including target, research areas, clinical information.
- High purity and quality validated by NMR and LC/MS.

Cell Death Series

Programmed cell death (PCD), referring to apoptosis, autophagy and programmed necrosis, is a tightly regulated cellular process that is central to the development, homeostasis and integrity of multicellular organisms. The dysregulation of programmed cell death is closely related to the occurrence and development of many human diseases such as cancer, immune diseases, neurodegenerative diseases and cardiovascular diseases.



Distinctive forms of programmed cell death and their morphological characteristics[1][2].

- HY-L051 22
  Ferroptosis Compound Library
- HY-L029 22
  Autophagy Compound Library
- HY-L003 22
  Apoptosis Compound Library
- HY-L059 22
  Pyroptosis Compound Library

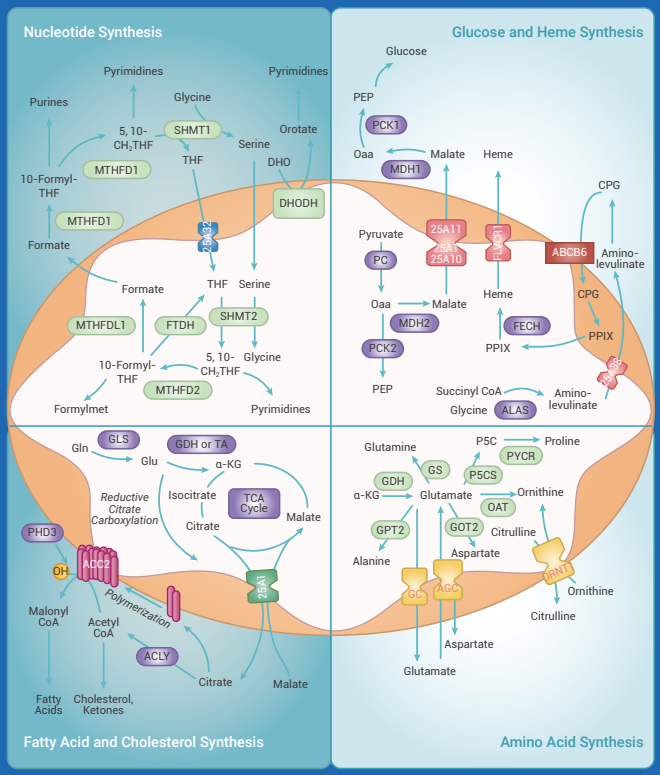
References: [1] Aging Dis. 2021 Feb 1;12(1):261-276. [2] J Cancer Sci Treatment. 2019 1(1): 17-24.

		HY-L051 **Ferroptosis Compound Library**	HY-L003 **Apoptosis Compound Library**	HY-L029 **Autophagy Compound Library**	HY-L059 **Pyroptosis Compound Library**
Morphological Features	Cell Membrane	Cell rounding	Cell rounding; membrane blebbing	Normal	Cell swelling; rupture of plasma membrane; bubbling;
	Cytoplasm	Smaller mitochondria; reduced mitochondria crista; elevated mitochondrial membrane densities; increased rupture of mitochondrial membrane	Apoptotic body formation	Accumulation of double-membraned autophagic vesicle	Release of inflammatory cellular contents
	Cell Nucleus	Normal	Smaller Nucleus; chromatin condensation; DNA damage	Normal	Moderate chromatin condensation; DNA damage
Biochemical Features		Iron metabolism and ROS production	Caspase activation; DNA fragment; ΔΨm dissipation	LC3-I to LC3-II conversion; p62 degradation	Inflammatory Caspase activation (CASP1, CASP3, and GSDMD)
Major Regulators		**Positive:** VDAC2/3, Ras, NOX, TFR1, p53, CARS	**Positive:** p53, Bax, Other Pro-Apoptotic Bcl-2 Family Proteins	**Positive:** ATG5, ATG7, Beclin 1	**Positive:** Caspase-1, Caspase-4, Caspase-5, Gasdermin D, NLRP3
		Negative: GPX4, SLC7A11	**Negative:** Bcl-2, Bcl-XL, Other Anti-Apoptotic Bcl-2 Family Proteins	**Negative:** mTOR	
Library Description		**600+** ferroptosis signaling pathway related compounds with ferroptosis-inducing or -inhibitory activity.	**1,500+** apoptosis-related compounds mainly focusing on the key targets in the apoptosis pathway.	**1,100+** autophagy-related compounds for the research of autophagy-related regulation and diseases	**800+** pyroptosis-related compounds focusing on the key targets in the pyroptosis pathway.
Main Targets in Library		GPX4, Lipoxygenase, HMG-CoA Reductase (HMGCR), Reactive Oxygen Species, Glutamylcysteine Synthetase, Iron Chelator, etc.	Bcl-2 Family, c-Myc, Caspase, FKBP, TNF Receptor, RIP Kinase, etc.	FKBP, LRRK2, ULK, etc.	Caspase-1, Caspase-4, Caspase-11, Caspase-3, Gasdermin D, NOD-Like Receptor (NLR), etc.
Library Features		• Bioactivity and safety have been confirmed in clinical trials and/or preclinical research for HTS and HCS, and some products have been approved by FDA for marketing. • More detailed compound information with structure, IC_{50}, and brief introduction. • High purity and quality validated by NMR and LC/MS.			

Metabolism Series

Metabolism is the set of life-sustaining chemical reactions in organisms. Metabolic pathways are enzyme-mediated biochemical reactions that lead to biosynthesis (anabolism) or breakdown (catabolism) of natural product molecules within a cell or tissue. The main metabolism in the body includes glucose metabolism, lipid metabolism and protein metabolism. Imbalances in metabolic activities have been found to be critical in a number of pathologies, such as diabetes, cardiovascular diseases and metabolic syndrome.

Metabolites are the products and intermediates of cellular metabolism which are usually small molecules. In the process of new drug discovery, metabolites have become an important source of lead compounds because of their safety and the diversity of biological activities. Microbial metabolites play important roles in the development of antibiotic products and non-antibiotic active compounds because of their species diversity and structural novelty.



Mitochondria are biosynthetic hubs.[1]

Reference: [1] Nat Cell Biol. 2018 Jul;20(7):745-754.

Cat. No.: HY-L012

Metabolism/Protease Compound Library

(96-/384-well plate)

Functioned as catalysts, enzymes are crucial to metabolism - they allow a reaction to proceed more rapidly - and they also allow the regulation of the rate of a metabolic reaction. Proteases control a great variety of physiological processes that are critical for life, including the **immune response, cell cycle, cell death, wound healing, food digestion**, and **protein and organelle recycling**. Imbalances in metabolic activities have been found to be critical in a number of pathologies, such as **cardiovascular diseases, inflammation, cancer, and neurodegenerative diseases**. Metabolites are the products and intermediates of cellular metabolism which are usually small molecules. In the process of new drug discovery, metabolites have become important sources of lead compounds because of their safety and diversity of biological activities.

Product Features

- **3,000+** compounds targeting metabolic pathways, such as **Carbohydrate metabolism, Lipid metabolism, Amino acid metabolism,** etc. A useful tool for HTS and HCS.
- Covers full range of targets, such as **PDE, Cytochrome P450, HMG-CoA Reductase, DPP4, Proteasome, HCV Protease, IDO, Cathepsin, MMP**, etc.
- Bioactivity and safety confirmed by clinical trials and/or preclinical research. Some have been approved by FDA.
- High purity and quality validated by NMR and LC/MS.

Cat. No.: HY-L064

Glutamine Metabolism Compound Library

(96-/384-well plate)

Glutamine is an important metabolic fuel that helps rapidly proliferating cells meet the increased demand for ATP, biosynthetic precursors, and reducing agents. Mounting evidences indicate that altered glutamine metabolism in cancer cells has critical roles in supporting **macromolecule biosynthesis**, **regulating signaling pathways,** and **maintaining redox homeostasis**, all of which contribute to cancer cell proliferation and survival. Thus, intervention in glutamine metabolic processes could provide novel approaches to improve cancer treatment.

Product Features

- **600+** glutamine metabolism-related small molecules for HTS and HCS.
- Covers the main targets in glutamine metabolism, such as glucose transporter, glutamate dehydrogenase, glutaminase, c-Myc, etc.
- Bioactivity and safety confirmed by clinical trials and/or preclinical research. Some compouds have been approved by FDA.
- High purity and quality validated by NMR and LC/MS.

Cat. No.: HY-L058

Glycolysis Compound Library

(96-/384-well plate)

Glycolysis is used by all cells in the body for energy generation. Most cancer cells exhibit increased glycolysis and use this metabolic pathway for generation of ATP as a main source of their energy supply. This phenomenon is known as the Warburg effect and is considered as one of the most fundamental metabolic alterations during malignant transformation. Because increased aerobic glycolysis is commonly seen in a wide spectrum of human cancers, developing novel glycolytic inhibitors as a new class of anticancer agents is likely to have broad therapeutic applications.

Product Features

- **500+** glycolysis-related small molecules for HTS and HCS.
- Covers the main targets, such as **hexokinase, glucokinase, enolase, pyruvate kinase, PDHK**, etc.
- Bioactivity and safety confirmed by clinical trials and/or preclinical research. Some compouds have been approved by FDA.
- High purity and quality validated by NMR and LC/MS.

Cat. No.: HY-L030

Human Endogenous Metabolite Compound Library

(96-/384-well plate)

The composition of endogenous metabolite compounds is affected by the upstream influence of the proteome and genome as well as environmental factors, lifestyle factors, medication, and underlying disease. Therefore, metabolites have been described as proximal reporters of disease because their abundances in biological specimens are often directly related to pathogenic mechanisms. In more recent years, metabolomics approach has been adopted or suggested to be used in various research areas including drug discovery, neurosciences, agriculture, food and nutrition, and environmental sciences.

Product Features

- **1,000+** human endogenous metabolites for HTS and HCS.
- All compounds are human endogenous metabolites with better bioavailability.
- A useful tool for metabolomics and metabolism-related drug discovery.
- Bioactivity and safety confirmed by clinical trials and/or preclinical research. Some compouds have been approved by FDA.
- High purity and quality validated by NMR and LC/MS.

Cat. No.: HY-L084

Microbial Metabolite Library

(96-/384-well plate)

Metabolites have become important sources of lead compounds in the development of new drugs due to their safety and diversity of biological activities. Microbial metabolites, in particular, play key roles in the development of antibiotic products and non-antibiotic active compounds due to their species diversity and structural novelty.

Product Features

- **600+** microbial metabolites that are important sources of lead compounds and can be used for HTS and HCS.
- A useful tool for metabonomics and metabolism-related drug discovery.
- Structurally diverse, bioactive, and cell permeable.
- High purity and quality validated by NMR and LC/MS.

Cat. No.: HY-L078

Gut Microbial Metabolite Library

(96-/384-well plate)

Accumulating evidence has revealed that intestinal microbiota plays an important role in human health and disease, including **cardiovascular diseases, inflammatory bowel disease, diabetes, obesity, cancer, depression**. Changes in the composition of gut microbiota associated with disease, called as dysbiosis, have been linked to pathologies. Indeed, the gut microbiome functions like the endocrine organ, generating bioactive metabolites which play important roles in human metabolism, health, and disease. Gut microbiome has become a novel therapeutic target for many diseases. Analysis and identification of gut microbial metabolites will contribute to the development of therapeutic methods.

Product Features

- **150+** gut microbial metabolites that can be used for HTS and HCS.
- All the compounds have good bioavailability.
- A useful tool for gut microbiome research and gut microbiome-related drug discovery.
- High purity and quality validated by NMR and LC/MS.

Cat. No.: HY-L091

Lipid Metabolism Compound Library

(96-/384-well plate)

Lipids are a fundamental class of organic molecules implicated in a wide range of biological processes, and based on this can be broadly classified into five categories: fatty acids, triacylglycerols (TAGs), phospholipids, sterol lipids and sphingolipids. Lipids play a crucial role in different metabolic pathways and cellular functions. Lipid metabolism is an important physiological process that is related to **nutrient adjustment, hormone regulation**, and **homeostasis**. Lipid metabolism dysregulation is associated with many diseases such as obesity, liver disease, aging, etc.

Product Features

- **300+** lipid metabolism-related compounds that can be used for both HTS and HCS.
- Covers key targets of lipid metabolism pathways, such as **acetyl-CoA Carboxylase, Fatty Acid Synthase (FASN), Lipoxygenase, and HMG-CoA Reductase (HMGCR),** etc.
- Bioactivity and safety confirmed by clinical trials and/or preclinical research. Some compounds have been approved by FDA.
- High purity and quality validated by NMR and LC/MS.

Cat. No.: HY-L092

Glucose Metabolism Compound Library

(96-/384-well plate)

Glucose homeostasis is tightly regulated to meet the energy requirements of the vital organs and maintain an individual's health. Glucose metabolism includes glycolysis, tricarboxylic acid cycle, pentose phosphate pathway, oxidative phosphorylation and other metabolic pathways. Glucose is the major carbon source that provides the main energy for life. Glucose metabolism dysregulation is also implicated in many diseases such as **diabetes, heart disease, neurodegenerative diseases** and even **cancers**.

Product Features

- **600+** glycometabolism-related compounds that can be used for both HTS and HCS.
- Covers the key targets in glucose metabolism pathways, such as **Isocitrate Dehydrogenase (IDH), Lactate Dehydrogenase, NADPH Oxidase, Glutathione Peroxidase,** etc.
- Bioactivity and safety confirmed by clinical trials and/or preclinical research. Some compounds have been approved by FDA.
- High purity and quality validated by NMR and LC/MS.

According to Product Features & Structures

Different physico-chemical properties of the products determine their characteristics and ultimately their applications in different research areas. For example, some compounds with low MW, fewer formal charges (particularly, negative charges) and lower polar surface area tend to be more CNS-penetrant. CNS-penetrant compounds are important tools for the study of neurological disorders, but they also have neurotoxicity[1] . Chemical probe, with high potency, selectivity and cell-permeability, play important roles in both fundamental and applied biological research. By analyzing the different properties of small molecule compounds, MCE can provide a variety of compound libraries with different properties, which you can choose according to your needs.

Different product structures determine different functions. For example, compounds with covalent reactive groups can bind irreversibly to target through covalent bonds which can lead to the development of highly selective inhibitors and overcome drug resistance[1]. Nucleoside and nucleotide analogues can mimic their physiological counterparts and subsequently be incorporated into DNA and RNA to inhibit cellular division and viral replication. Nucleoside and nucleotide analogues can be used to inhibit cancer cell growth, viral replication as well as other indications.

Reference: [1] Proc Natl Acad Sci U S A. 2005 May 24;102(21):7665-70.

Product Name	Compound Number	Product Features
HY-L028 CNS-Penetrant Compound Library	600+	• A unique collection of bioactive CNS-penetrant compounds. • A useful tool for the discovery of drugs used for brain diseases, such as **brain tumors, mental disorders, and neurodegenerative diseases**.
HY-L023 Toxins for Antibody-Drug Conjugate Research Library	40+	• Structurally diverse, including **Auristatin derivatives, Maytansinoids, Calicheamicin, Duocarmycin, Pyrrolobenzodiazepines (PBDS)**.
HY-L061 Orally Active Compound Library	2,500+	• A unique collection of compounds for discovering new drugs with **oral bioavailability**. • All compounds with confirmed oral activity.
HY-L063 Chemical Probe Library	300+	• A unique collection of chemical probes with high potency, selectivity and cell-permeability. • A useful tool for fundamental biological research and drug discovery.
HY-L076 Drug-Induced Liver Injury (DILI) Compound Library	1,000+	• A unique collection of hepatotoxic compounds. • Including **antibiotics, anti-cancer agents, anti-inflammatory** agents. • Including several different toxicities: **steatosis, mitochondrial toxicity, cholestasis, drug allergy (hypersensitivity)**.
HY-L094 Food-Sourced Compound Library	1,600+	• All the compounds can be derived from food, which have certain safety. • All products are provided with detailed food sources. • Structurally diverse, bioactive, and cell permeable.
HY-L093 Food Additive Library	400+	• All compounds are approved food additives. An important source of lead compounds. • Structurally diverse, bioactive, and cell permeable.
HY-L033 Peptidomimetic Library	400+	• A unique collection of compounds that act as substitutes for peptides in their interaction with receptors for drug discovery. • **Peptoid, α-helix mimetics, β-turn/sheets mimetics** and compounds target **protein-protein interactions** are included.

Product Name	Compound Number	Product Features
HY-L036 Covalent Screening Library	1,500+	• A unique collection of compounds including molecules identified as covalent inhibitors and other bioactive molecules having common covalent warheads. • Structurally diverse, a variety of covalent warheads, such as **acrylamide, alkyl halides, epoxides, azacyclic amines, disulfide**, etc.
HY-L036P Covalent Screening Library Plus	3,000+	• HY-L036P possesses a more powerful screening capability, a complement to HY-L036 by adding some fragment compounds with covalent warheads.
HY-L041 Macrocyclic Compound Library	200+	• A useful tool for the discovery of "**undruggable**" targets such as **protein-protein interactions (PPIs)** inhibitors. • Cyclopeptides, crown ethers, calixarene and so on are included.
HY-L042 Glycoside Compound Library	300+	• **O-glycosides, Ester glycosides, thioglycosides, N-glycoside, sugar-like** compounds are included.
HY-L043 Lipid Compound Library	400+	• A unique collection of lipid and lipid derivative related compounds. • Structurally diverse, **triglycerides, phospholipids,** sphingolipids, steroids and their structural analogues or derivatives are included.
HY-L044 Nucleotide Compound Library	300+	• A unique collection of **nucleotide/nucleoside** and **nucleotide/nucleoside** analogue compounds. • A useful tool for discovering anti-cancer and antiviral drugs.

Publications Citing Use of MCE Products in These Libraries

Autophagy. 2021 Jun;17(6):1426-1447.

Cell Death Dis. 2021 Mar 3;12(3):229.

Cancer Lett. 2020 Jul 1;481:15-23.

Sci Adv. 2020 Jul 17;6(29):eaba1593.

Cancer Res. 2021 Jun 1;81(11):3105-3120.

Cancer Lett. 2021 Mar 16;S0304-3835(21)00117-8.

Nat Cell Biol. 2020 Oct;22(10):1187-1196.

Cell Death Dis. 2020 Sep 15;11(9):754.

Cat. No.: HY-L032

Fragment Library

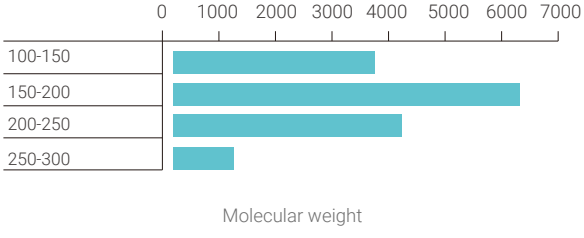
(96-/384-well plate)

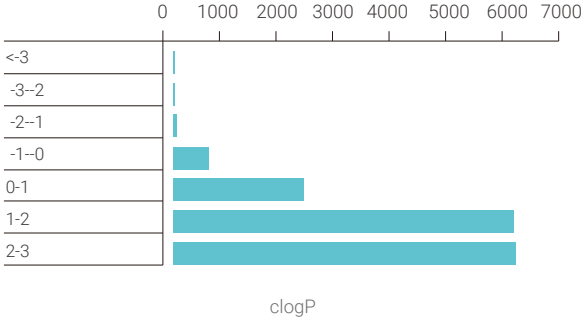
Fragment-based drug discovery (FBDD) is well suited for discovering both drug leads and chemical probes of protein function. It can cover broad areas of chemical space and allows the use of creative chemistry. Fragment-based drug discovery is well-established in industry and has resulted in a variety of drugs entering clinical trials, with two, vemurafenib and venetoclax, already approved. FBDD also has key attractions for academia. Notably, it is able to engage difficult or novel targets for which no chemical matter may be found in existing HTS collections.

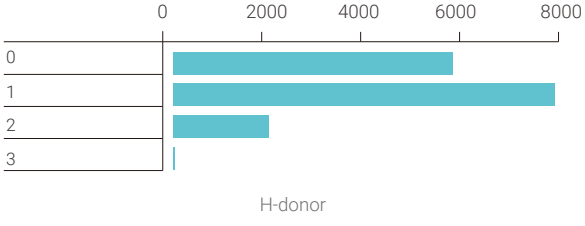
Product Features

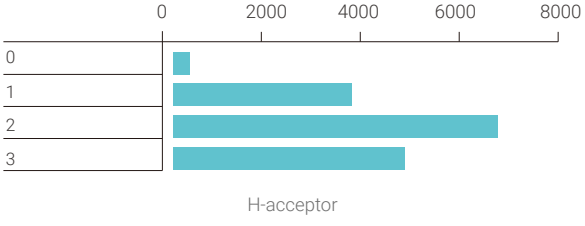
- **16,000+** fragment compounds for fragment-based drug discovery (FBDD).
- All compounds follow the Rule of "Three", in which molecular weight ≤300 Da, the number of hydrogen bond donors (H-donors) ≤3, the number of hydrogen bond acceptors (H-acceptors) is ≤3 and cLogP is ≤3.
- Diversified structures, covering a broader chemical space.
- The solubility of most products in DMSO can reach more than **200 mM**. Higher concentration is also available.
- High purity and quality validated by NMR and LC/MS.

Parameters







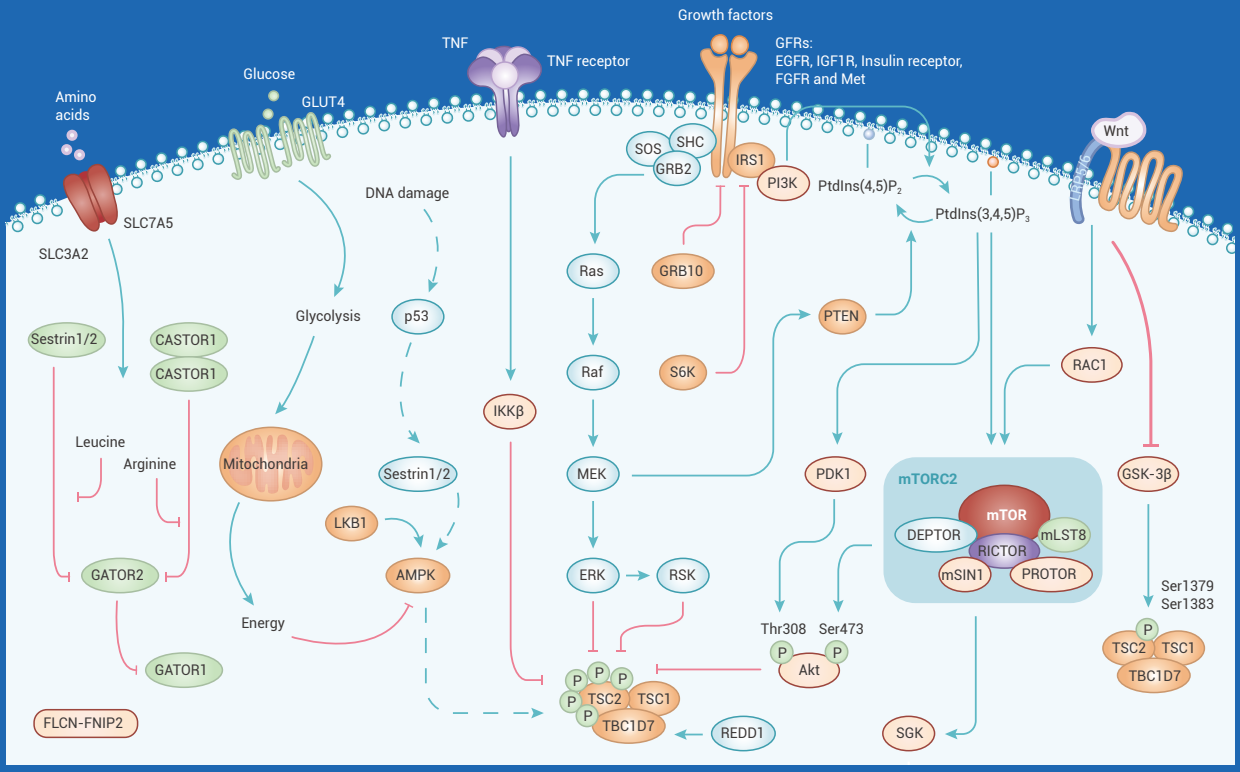


According to Signaling Pathway or Protein Family

Signal transduction or cell signaling concerns the mechanisms by which biological information is transferred between cells or inside the cell. The responses to the extracellular signal are generated by diverse signal transduction mechanisms that frequently involve small intracellular molecules (second messengers) that transmit signals from activated receptors to the cell interior, resulting in changes in the expression of genes and the activity of enzymes. These intercellular and intracellular signaling pathways are essential to the growth, development, metabolism, and the behavior of the organism[1].

Cell signaling pathways are involved in the pathophysiology of many diseases. The mutations, molecular damage or functional change of the proteins in the signaling pathway will cause diseases. Knowledge of basic cell signaling mechanisms is therefore essential to understand pathophysiologic and pharmacologic mechanisms.

Reference: [1] Encyclopedia of Respiratory Medicine. 2006,Pages 10-18,ISBN 9780123708793.



Product Name	Compound Number	Product Features
HY-L037 Antioxidants Compound Library	800+	• Act as antioxidants for HTS and HCS. • **Main targets**: NF-κB, mTOR, Keap1-Nrf2, AMPK, Sirtuin, etc.
HY-L038 Differentiation Inducing Compound Library	1,000+	• Act as stemness/self-renewal pathway inhibitors and differentiation activators/agonists. • **Main targets**: Wnt/β-catenin, Hedgehog/Gli, Jagged/Notch, BMP and retinoic acid (RA), etc.
HY-L039 Reprogramming Compound Library	1,300+	• A unique collection of reprogramming compounds. • **Main targets**: Epigenetic modifiers, metabolism regulators, cell senescence alleviators and signaling pathway modulators such as Wnt, MET, Hedgehog pathways.
HY-L050 Ubiquitination Compound Library	200+	• A unique collection of bioactive ubiquitination related compounds. • **Main targets**: Proteasome, E1/E2/E3 Enzyme, Deubiquitinase, p97, etc.
HY-L004 Cell Cycle/DNA Damage Compound Library	1,200+	• A unique collection of Cell Cycle/DNA Damage related compounds. • **Main targets**: CDK, ROCK, Aurora Kinase, ATM/ATR, DNA-PK, DNA/RNA Synthesis, etc.
HY-L005 Epigenetics Compound Library	800+	• A unique collection of compounds used for epigenetics research and associated assays. • **Main targets**: HDAC, Histone Demethylase, HAT, DNMT, Epigenetic Reader Domain, MicroRNA, etc.
HY-L006 GPCR/G Protein Compound Library	1,600+	• A unique collection of compounds targeting GPCRs for various research and drug development projects. • **Main targets**: 5-HT Receptor, Dopamine Receptor, Opioid Receptor, Adrenergic Receptors, Cannabinoid Receptor, mGluR, ETA Receptor, etc.
HY-L024 Histone Modification Research Compound Library	400+	• A unique collection of bioactive compounds related to histone modification. • **Main targets**: Epigenetic Reader Domain, HDAC, HAT, Histone Demethylase, Histone Methyltransferase, Sirtuin, etc.

Product Name	Compound Number	Product Features
HY-L007 Immunology/Inflammation Compound Library	3,000+	• A unique collection of bioactive compounds used for Immunology/Inflammation research. • **Main targets**: CCR, COX, Interleukin Related, IRAK, MyD88, PDE, PD-1/PD-L1, TLR, etc.
HY-L008 JAK/STAT Compound Library	300+	• A unique collection of bioactive compounds related to JAK/STAT signaling. • **Main targets**: JAK, STAT, EGFR, Pim, etc.
HY-L009 Kinase Inhibitor Library	2,000+	• A unique collection of kinase inhibitors. • **Main targets**: Protein Kinases (VEGFR, EGFR, BTK, CDK, Akt, etc.), lipid kinases (PI3K, PI4K, SK, etc.) and Hexokinase.
HY-L010 MAPK Compound Library	300+	• A unique collection of MAPK signaling pathway inhibitors or activators. • **Main targets**: ERK, JNK, MEK, p38 MAPK, Raf, RSK, etc.
HY-L011 Membrane Transporter/Ion Channel Compound Library	1,000+	• A unique collection of compounds related to Ion Channel and Membrane Transporter research. • **Main targets**: Pgp, CRM1, BCRP, etc., and Ion Channels including CFTR, proton pump, sodium pump, calcium pump, etc.
HY-L013 Neuronal Signaling Compound Library	1,700+	• A unique collection of neuronal signaling pathways-related compounds. • **Main targets:** 5-HT Receptor, AChE, AMPAR, Beta-secretase, Dopamine Receptor, Melatonin Receptor, AChR, Opioid Receptor, γ-secretase, etc.
HY-L014 NF-κB Signaling Compound Library	500+	• A unique collection of NF-κB signaling pathways related compounds. • **Main targets**: IKK, Keap1-Nrf2, NF-κB, etc.
HY-L015 PI3K/Akt/mTOR Compound Library	400+	• A unique collection of compounds used for PI3K/Akt/mTOR pathways research. • **Main targets**: Akt, AMPK, DNA-PK, PDK-1, mTOR, PI3K, PTEN, etc.
HY-L016 Protein Tyrosine Kinase Compound Library	700+	• A unique collection of protein kinase inhibitors or activators. • **Main targets**: VEGFR, ALK, Btk, Bcr-Abl, c-Met/HGFR, EGFR, FGFR, Insulin Receptor, JAK, PDGFR, etc.

Product Name	Compound Number	Product Features
HY-L017 Stem Cell Signaling Compound Library	1,200+	• A unique collection of compounds related to stem cell regulatory and signaling pathways research. • **Main targets**: GSK-3, Hedgehog, Notch, JAK, ROCK, Wnt, γ-secretase, Casein Kinase, etc.
HY-L018 TGF-beta/Smad Compound Library	150+	• A unique collection of TGF-beta/Smad inhibitors or activators. • **Main targets**: PKC, ROCK, TGF-beta/Smad, TGF-β Receptor, etc.
HY-L045 Oxygen Sensing Compound Library	1,600+	• A unique collection of oxygen sensing related compounds. • **Main targets**: HIF, HIF Prolyl-Hydroxylase, E1/E2/E3 Enzyme, ROS, PI3K, MAPK, etc.
HY-L054 Endoplasmic Reticulum Stress Compound Library	150+	• A unique collection of ER stress-related compounds. • **Main targets**: PERK, IRE1, ATF6, etc.
HY-L020 Wnt/Hedgehog/Notch Compound Library	200+	• A unique collection of compounds used for Wnt/Hedgehog/Notch pathway research and screening. • **Main targets**: Notch, Gli, GSK-3, Hedgehog, Porcupine, sFRP-1, Smo, Wnt, β-catenin, etc.
HY-L060 Cytoskeleton Compound Library	900+	• A unique collection of compounds used for cytoskeleton research. • **Main targets**: Kinesin, Microtubule/Tubulin, Arp2/3 Complex, Bcr-Abl, etc.
HY-L062 Neurotransmitter Receptor Compound Library	1,200+	• A unique collection of compounds used for neurological diseases research. • **Main targets**: Neurotransmitter receptors including mAChR, nAChR, Adrenergic Receptor, Dopamine Receptor, etc.
HY-L089 Mitochondria-Targeted Compound Library	400+	• A unique collection of compounds against mitochondrial protein targets. • **Main targets**: Mitochondrial Metabolism, ATP Synthase, Mitophagy, Reactive Oxygen Species, etc.

Product Name	Compound Number	Product Features
HY-L072 Exosomes Compound Library	50+	• A unique collection of Exosomes secretion-related compounds. • **Main targets**: N-SMase, PIKfyve, etc.
HY-L090 Transcription Factor Targeted Library	800+	• A unique collection of compounds with validated transcription factor targets modulating properties. • **Main targets**: STAT, c-Myc, Oct3/4, NF-κB, etc.
HY-L081 Phosphatase Inhibitor Library	100+	• A unique collection of phosphatase inhibitors for HTS and HCS. • **Main targets**: PTPs and serine/threonine-specific protein phosphatases (PP1, PP2A, and PP2B, etc.).
HY-L088 Angiogenesis Related Compound Library	1,300+	• A unique collection of compounds with validated angiogenesis targets modulating properties. • **Main targets**: VEGFR, Ephrin Receptor, PDGFR, FGFR, etc.

Publications Citing Use of MCE Products in These Libraries

Cell. 2021 Apr 15;184(8):2,167-2182.e22.

Cancer Res. 2021 Apr 5;canres.3738.2020.

Nat Commun. 2021 Jul 21;12(1):4441.

Sci Adv. 2021 Apr 14;7(16):eabb2213.

Front Cell Dev Biol. 2021 Sep 20;9:712224.

Elife. 2021 Sep 29;10:e65811.

Cell Rep. 2021 Jul 20;36(3):109404.

Small. 2020 Jun;16(22):e2,001371.

Mil Med Res. 2020 Sep 6;7(1):42.

Cancer Biol Med. 2020 Aug 15;17(3):707-725.

Cancer Res. 2021 Jun 1;81(11):3105-3120.

Autophagy. 2021 Jun;17(6):1426-1447.

Nat Protoc. 2021 Jan;16(1):405-430.

Cell Prolif. 2021 Jan;54(1):e12932.

Elife. 2021 Jun 16;10:e63104.

Toxins. 2021 Aug 22;13(8):585.

Life Sci. 2020 Sep 1;256:117983.

Cell Death Differ. 2020 Jul;27(7):2158-2175.

Curr Biol. 2020 Nov 2;30(21):4128-4141.e5.

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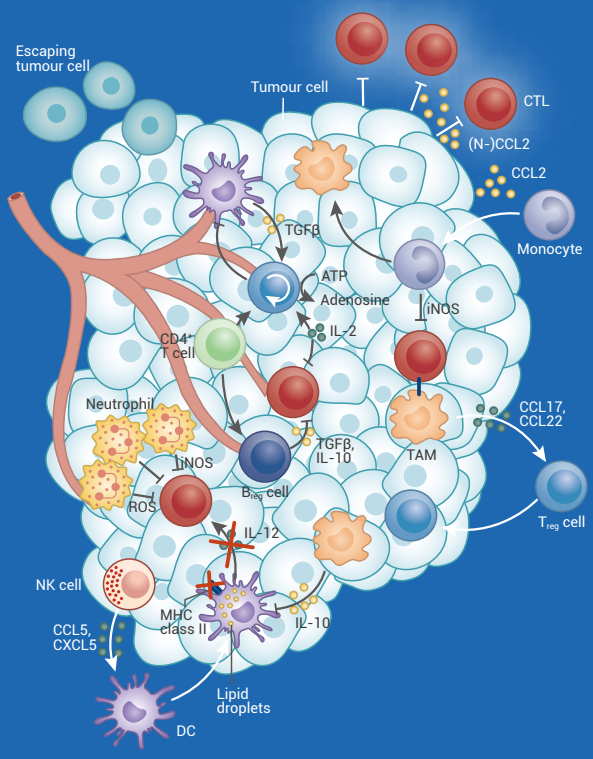
Anti-Cancer Series

Cancer is the second leading cause of death worldwide and a serious threat to human health. Dysregulation of cell cycle and cell division are the main causes of cancer. In cancer treatment, the commonly used treatment methods include chemotherapy, radiotherapy, targeted therapy, immunotherapy, surgical treatment or a combination of several treatments. Chemotherapy, as a traditional method of cancer treatment, has high side effects. In recent years, targeted therapy and tumor immunity have gradually become important means of cancer treatment. Targeted therapies play an important role in cancer treatment by targeting proteins that control the growth, division and spread of cancer cells. Tumor immunotherapy is a treatment method to eliminate tumors by activating and mobilizing the body's immune system to kill tumor cells. Immune checkpoint is a common target in tumor immunotherapy. In recent years, more and more studies have shown that tumor microenvironment plays an increasingly important role in the development of tumor, especially in the study of tumor immunity and tumor metabolism.



The immunosuppressive tumour microenvironment [1]

Reference: [1] Nat Rev Immunol. 2020 Aug;20(8):483-497.

Cat. No.: HY-L025

Anti-Cancer Compound Library

(96-/384-well plate)

Cancer is the second leading cause of death globally and seriously threatens human health. A neoplasm and malignant tumor are other common names for cancer. Disruption of the normal regulation of cell-cycle progression and division lies at the heart of the events leading to cancer. Targeted therapy, which targets proteins that control how cancer cells grow, divide and spread, plays an important role in cancer treatment. Recent studies mainly focus on targeting the key proteins for cancer surviving, cancer stem cells, the tumor microenvironment and tumor immunology, etc.

Product Features

- **5,000+** compounds with **anti-solid tumor** and/or **hematologic tumor** activity, which can be used for both HTS and HCS.
- Covers diverse signaling pathways, including **kinase, GPCR, epigenetics** and other hot research areas.
- Bioactivity and safety have been confirmed by clinical trials and/or preclinical research. Some compounds have been approved by FDA.
- High purity and quality validated by NMR and LC/MS.

Examples of Targets in Anti-Cancer Compound Library

≥100 29-99 0-28

- ADC Cytotoxin
- Androgen Receptor
- Autophagy
- Calcium Channel
- c-Kit
- Deubiquitinase
- EGFR
- Estrogen Receptor/ERR
- FLT3
- Histone Acetyltransferase
- IDO
- MDM-2/p53
- Mitophagy
- Notch
- Raf
- Reactive Oxygen Species
- Akt
- Antibiotic
- Bcl-2 Family
- Casein Kinase
- c-Met/HGFR
- DNA Alkylator/ Crosslinker
- GSK-3
- Histone Demethylase
- HSP
- JAK
- MEK
- MMP
- Nucleoside Antimetabolite/Analog
- RET
- ALK
- Apoptosis
- Bcr-Abl
- Caspase
- COX
- DNA/RNA Synthesis
- Epigenetic Reader Domain
- Ferroptosis
- HDAC
- Histone Methyltransferase
- JNK
- Microtubule/Tubulin
- mTOR
- p38 MAPK
- ROCK
- RAR/RXR
- AMPK
- Aurora Kinase
- Btk
- CDK
- Cytochrome P450
- E1/E2/E3 Enzyme
- ERK
- FGFR
- HIF/ HIF Prolyl-Hydroxylase
- Keap1-Nrf2
- Mitochondrial Metabolism
- NF-κB
- PARP
- Ras
- Sirtuin
- Src

Cat. No.: HY-L031

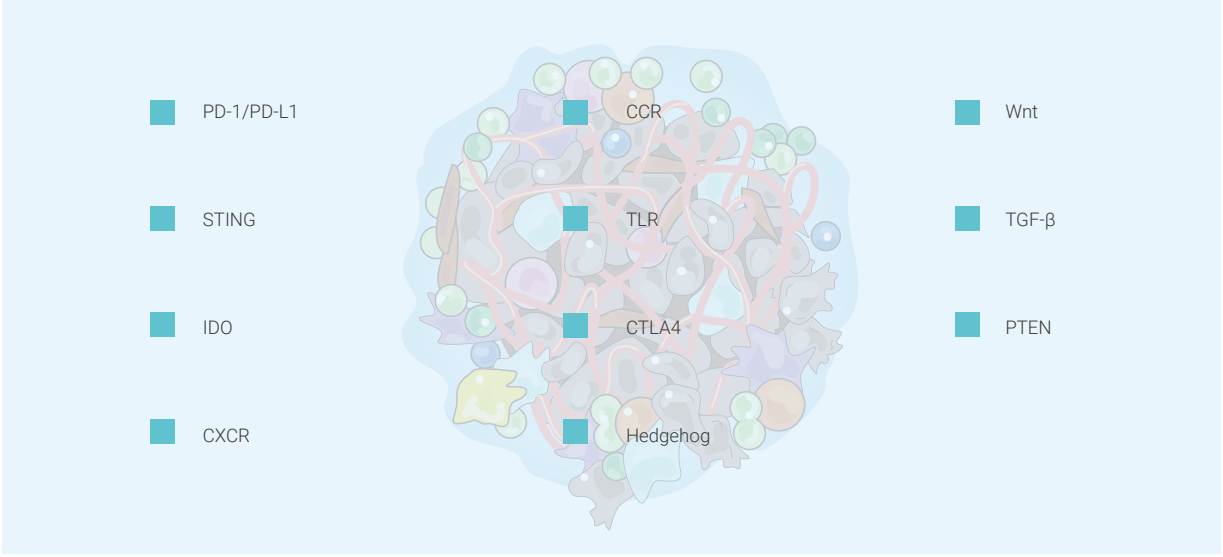
Small Molecule Immuno-Oncology Compound Library
(96-/384-well plate)

Immuno-Oncology is a type of immunotherapy that has the specific way of treating cancer. It works by stimulating our immune system to fight back. Normally, our immune system is able to destroy cancer cells in our body, however sometimes cancer cells can adapt and mutate, effectively hiding from our immune system. This is when tumors can develop and become a threat to our health. Immuno-oncology involves mobilizing lymphocytes to recognize and eliminate cancer cells using the body's immune system. There are several immuno-oncology treatments available, including **Immune cell therapy (CAR-T), monoclonal antibodies (mABs)** and **checkpoint inhibitors, cytokines** and cancer vaccines.

Product Features

- **300+** bioactive tumor immunology compounds that target some important checkpoints such as **PD1/PD-L1, CXCR, Sting, IDO, TLR,** etc.
- A useful tool for cancer research by activation of antitumor immune response.
- Bioactivity and safety confirmed by clinical trials and/or preclinical research. Some compounds have been approved by FDA.
- Detailed compound information with structure, target and brief introduction.
- High purity and quality validated by NMR and LC/MS.

Examples of Targets in Small Molecule Immuno-Oncology Compound Library

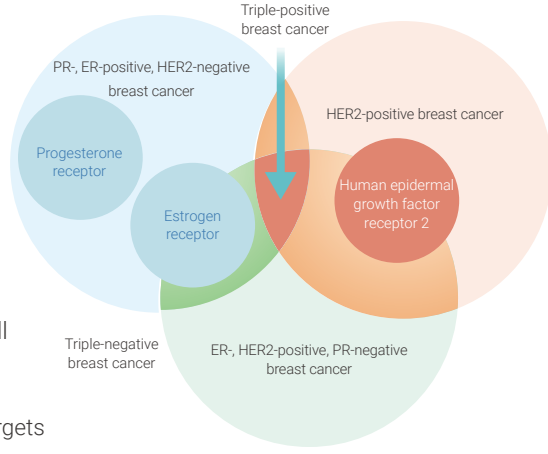


Cat. No.: HY-L074

Anti-Breast Cancer Compound Library

(96-/384-well plate)

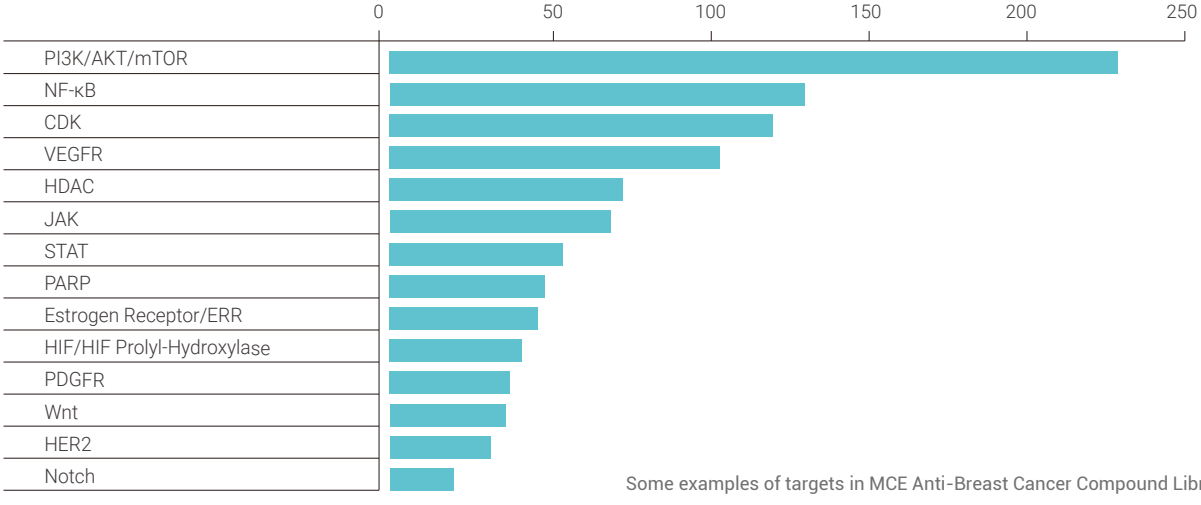
Breast cancer is the most frequent cancer among women, impacting 2.1 million women each year, and also causes the greatest number of cancer-related deaths among women. Breast cancer is a heterogeneous disease, which is categorized into 3 major subtypes based on the presence or absence of molecular markers for estrogen or progesterone receptors and human epidermal growth factor 2 (ERBB2; formerly HER2): hormone receptor positive/ERBB2 negative (70% of patients), ERBB2 positive (15%-20%), and triple-negative (tumors lacking all 3 standard molecular markers; 15%).



HER2, Estrogen Receptor, CDK, VEGFR, PI3K are commonly used targets in breast cancer treatment and are also important targets in anti-breast cancer drug discovery.

Product Features

- According to the analysis of the clinical and approved drugs used in breast cancer treatment, the targets commonly used in the treatment of breast cancer are collected. Based on these targets, MCE carefully collects **1,300+** compounds that have potential anti-breast cancer activity.
- Mainly target **EGFR, VEGFR, Estrogen Receptor, PI3K, AKT, JAK, STAT, PD-1/PD-L1**, etc.
- Bioactivity and safety have been verified by clinical trials and/or preclinical research. Some products have been approved by FDA.
- Detailed compound information with structure, target and brief introduction.
- High purity and quality validated by NMR and LC/MS.

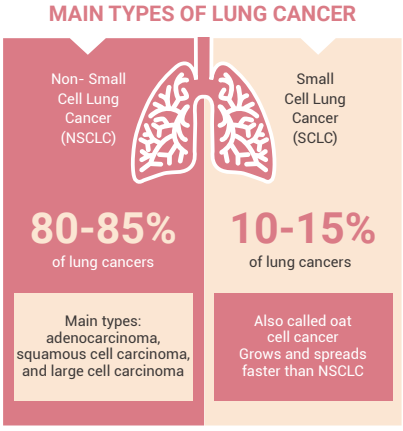


Some examples of targets in MCE Anti-Breast Cancer Compound Library

Cat. No.: HY-L075

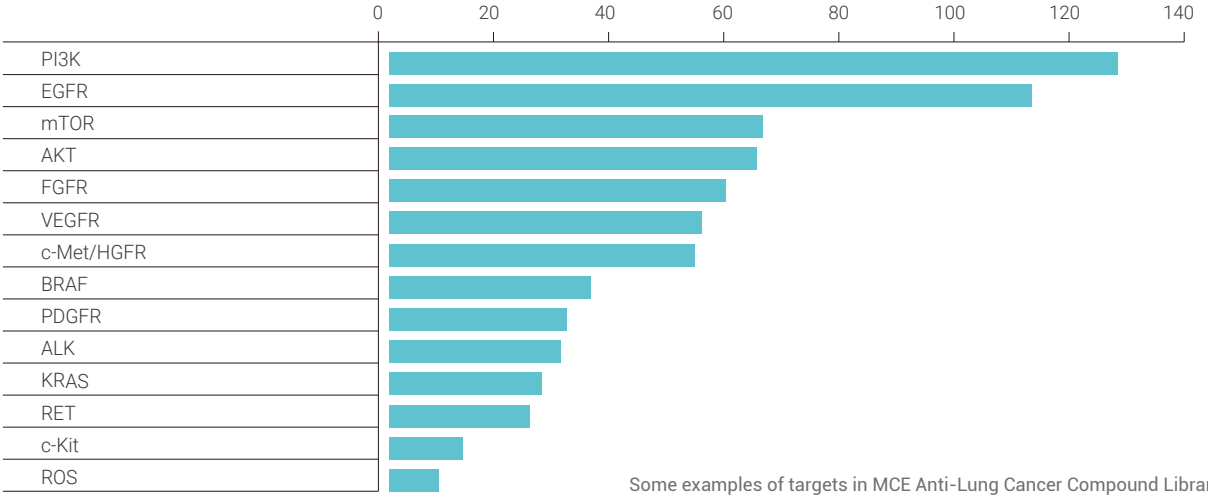
Anti-Lung Cancer Compound Library
(96-/384-well plate)

Lung cancer is a major global health problem, as it is the leading cause of cancer-related deaths worldwide. Lung cancer may be treated with surgery, chemotherapy, radiation therapy, targeted therapy, immunotherapy or a combination thereof. Targeted therapy is one of the most exciting developments in lung cancer medicine, especially for NSCLC. Extensive genomic characterization of NSCLC has led to the identification of molecular subtypes of NSCLC that are oncogene addicted and exquisitely sensitive to targeted therapies. These include activating mutations in epidermal growth factor receptor (EGFR) and BRAF or echinoderm microtubule-associated protein-like 4 (EML4)-anaplastic lymphoma kinase (ALK) fusions and ROS1 receptor tyrosine kinase fusions. These are important targets for targeted therapy.



Product Features

- According to the analysis of the clinical and approved drugs used in lung cancer treatment, the targets commonly used in the treatment of lung cancer are collected. Based on these targets, we carefully collect **1,200+** compounds that have potential anti-lung cancer activity.
- Mainly target **EGFR, VEGFR, Estrogen Receptor, PI3K, AKT, JAK, STAT, PD-1/PD-L1,** etc.
- Bioactivity and safety have been verified by clinical trials and/or preclinical research. Some products have been approved by FDA.
- High purity and quality validated by NMR and LC/MS.



Some examples of targets in MCE Anti-Lung Cancer Compound Library

Cat. No.: HY-L077

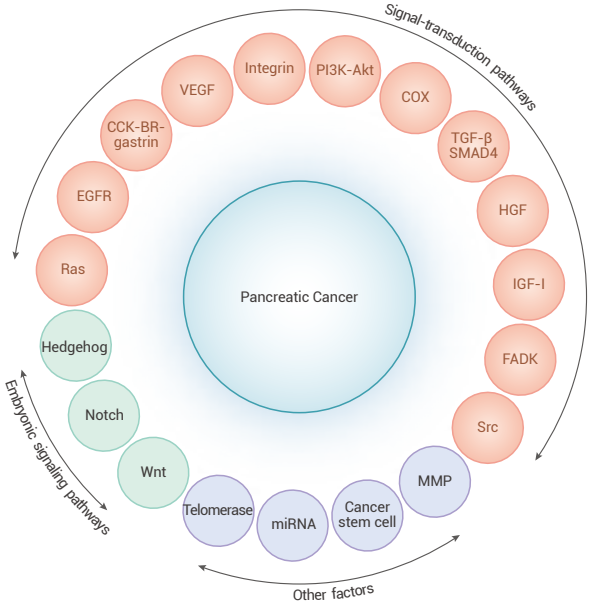
Anti-Pancreatic Cancer Compound Library

(96-/384-well plate)

Pancreatic cancer is a devastating disease with a low overall survival rate. Chemotherapy is the most common treatment for patients presenting with advanced pancreatic cancer. More recently, the era of targeted therapies has generated a lot of interest in discovering better approaches for patients with pancreatic cancer. Commonly mutated genes in pancreatic cancer include K-ras (in 74-100% of cases), p16INK4a (up to 98%), p53 (43 to 76%), DPC4 (about 50%), HER-2/neu (in about 65%) and FHIT (found in 70% of cases). Other genes include notch1, Akt-2, BRCA2 and COX-2. These proteins are important targets of target therapies for pancreatic cancer.

Product Features

- According to the analysis of the clinical and approved drugs used in pancreatic cancer treatment, the targets commonly used in the treatment of pancreatic cancer are collected. Based on these targets, MCE carefully collects **1,600+** compounds that have potential anti-pancreatic cancer activity.
- Mainly target **EGFR, ALK, ROS1, c-MET/HGFR, RET, FGFR**, etc.
- Bioactivity and safety have been verified by clinical trials and/or preclinical research. Some products have been approved by FDA.
- High purity and quality validated by NMR and LC/MS.



Some examples of targets in MCE Anti-Pancreatic Cancer Compound Library

Cat. No.: HY-L079

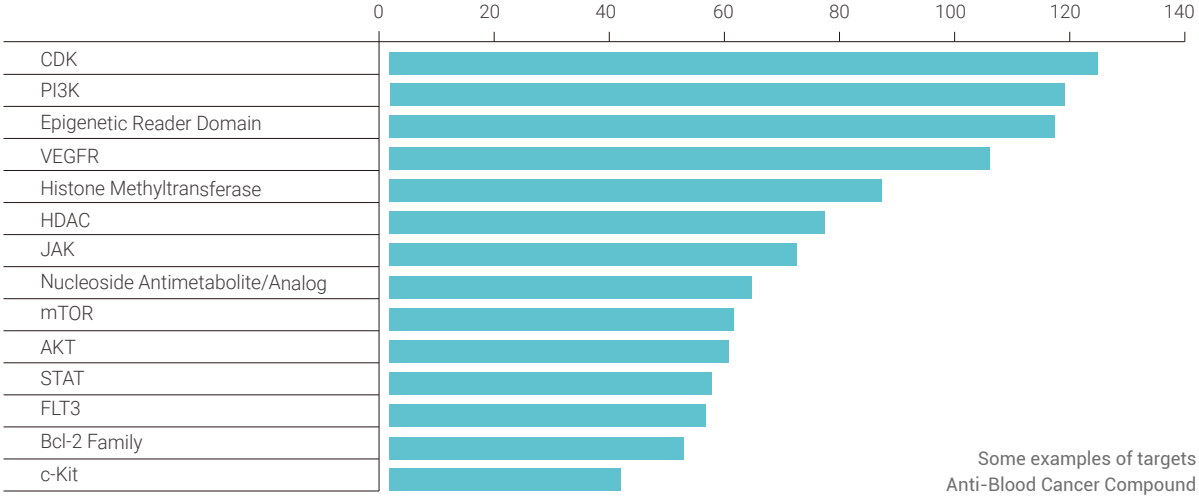
Anti-Blood Cancer Compound Library

(96-/384-well plate)

Blood cancers, also called hematologic cancers, occur when abnormal blood cells start growing out of control, interrupting the function of normal blood cells, which fight off infection and produce new blood cells. Most blood cancers start in the bone marrow, which is where blood is produced. There are three main types of blood cancers: leukemia, lymphoma and myeloma, which afflict millions of children and adults every year, and are often deadly.

Product Features

- According to the analysis of the clinical and approved drugs used in blood cancer treatment, the targets commonly used in the treatment of blood cancer are collected. Based on these targets, MCE carefully collects **1,800+** compounds that have potential anti-blood cancer activity.
- Mainly target **EGFR, ALK, ROS1, c-MET /HGFR, RET, FGFR**, etc.
- Bioactivity and safety have been verified by clinical trials and/or preclinical research. Some products have been approved by FDA.
- Detailed compound information with structure, target and brief introduction.
- High purity and quality validated by NMR and LC/MS.



Some examples of targets in MCE Anti-Blood Cancer Compound Library

Publications Citing Use of MCE Products in This Library

J Exp Clin Cancer Res. 2021 Sep 22;40(1):297.
Cancer Sci. 2021 Mar;112(3):997-1010.
Mol Cancer Ther. 2020 Mar;19(3):906-919.
J Immunother Cancer. 2021 Jul;9(7):e001758.
Biochem Pharmacol. 2020 Aug;178:114103.
Cell Mol Immunol. 2020 May;17(5):496-506.
Theranostics. 2021 Mar 24;11(12):5650-5674.
J Med Chem. 2020 Aug 13;63(15):8380-8387.

Cat. No.: HY-L080

Targeted Therapy Drug Library

(96-/384-well plate)

Targeted cancer therapies are drugs or other substances that block the growth and spread of cancer by interfering with specific molecular targets that are involved in the growth, progression, and spread of cancer.There are several different types of targeted therapy. The most common types are small-molecule drugs and monoclonal ant ibodies. Because of high specificity, low side effects and potent anticancer activity, targeted therapy has become the mains tream of new anti-tumor drugs. Various targeted therapies have been approved by FDA and used in the treatment of diseases.

Product Features

- A unique collection of **100+** approved targeted therapeutic small molecule drugs which can be used for HTS and HCS.
- Mainly target **EGFR, Bcr-Abl, ALK, JAK, Epigenetics**, etc.
- Bioactivity and safety have been verified by clinical trials and/or preclinical research. Some products have been approved by FDA.
- High purity and quality validated by NMR and LC/MS.

Cat. No.: HY-L083

Anti-Cancer Metabolic Compounds Library

(96-/384-well plate)

The paramount hallmark of tumor metabolism is “aerobic glycolysis” or the Warburg effect, coined by Otto Warburg in 1926, in which cancer cells produce most of energy from glycolysis pathway regardless of whether in aerobic or anaerobic condition. Usually, cancer cells are highly glycolytic and take up more glucose than do normal cells from outside. The increased uptake is facilitated by the overexpression of several isoforms of membrane glucose transport-ers (GLUTs). Likewise, the metabolic pathways of glutamine, amino acid and fat metabolism are also altered. Recent trends suggest that targeting the altered metabolic pathways of cancer cells result in energy crisis inside the cancer cells and can selectively inhibit cancer cell proliferation by delaying or suppressing tumor growth.

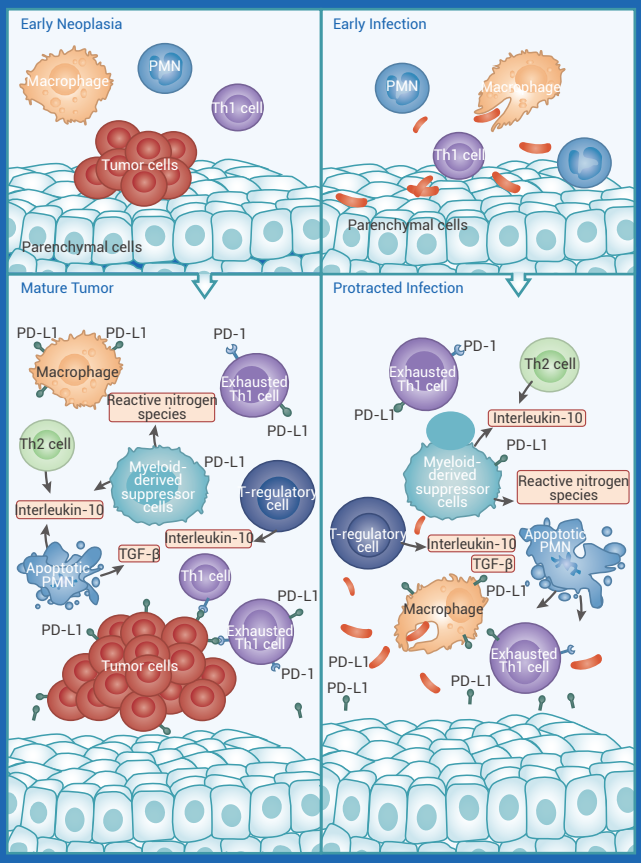
Product Features

- A unique collection of **800+** tumor metabolism-related small molecule compounds, which can be used for anti-cancer metabolism targets identification, validation as well as anti-cancer drug discovery.
- Covers various signaling pathways and targets related to tumor metabolism, such as **glucose metabolism, glutamine metabolism, amino acid metabolism, fat metabolism**, etc.
- Bioactivity and safety have been verified by clinical trials and/or preclinical research. Some products have been approved by FDA.
- High purity and quality validated by NMR and LC/MS.

Anti-Infection Series

An infection occurs when another organism enters a person's body and causes disease. The organisms that cause infections are very diverse and can include things like viruses, bacteria, fungi, and parasites. The immune system is an effective barrier against infectious agents.

MCE provides a unique collection of anti-infective compounds with detailed classification by anti-bacterial, anti-viral, anti-fungal and anti-parasite activities. You can choose based on your need:



Immune Phenotypes of Cancer and Protracted Infection.[1]

Reference: [1] N Engl J Med. 2014 Jul 24;371(4):380-3.

Cat. No.: HY-L002

Anti-Infection Compound Library

(96-/384-well plate)

An infection occurs when another organism enters a person's body and causes disease. The organisms that cause infections are very diverse and can include things like viruses, bacteria, fungi, and parasites. The immune system is an effective barrier against infectious agents.

Product Features

- **1,800+** bioactive anti-infection (**anti-bacteria, anti-fungi, anti-parasite and anti-virus**) compounds that could be used for HTS and HCS.
- Structurally diverse, medicinally active, and cell-permeable.
- Bioactivity and safety have been confirmed by clinical trials and/or preclinical research. Some compounds have been approved by FDA.
- Detailed bioactivity information, including target, research areas, clinical information.
- High purity and quality validated by NMR and LC/MS.

Cat. No.: HY-L027

Antiviral Compound Library

(96-/384-well plate)

Viruses, much simpler organisms than bacteria, are made from protein substances and nucleic acid. Even though the exact mechanism of infection is extremely specific to each type of virus, the general scheme of infection can be represented in the following manner: A virus is absorbed on the surface of a host cell and then permeates through the membrane, where it releases nucleic acid from its protein protection. Then the viral nucleic acid begins to replicate, and transcription of the viral genome takes place either in the cytoplasm or in the nucleus of the host cell. As a result of these events, a large amount of viral nucleic acid and protein are made to make new generations of virions. Therefore, one mechanism of action of antiviral drugs is to interfere with the ability of a virus to get into a target cell. The second mechanism is to target the processes that synthesize virus components after a virus invades a cell, such as a nucleotide or nucleoside analogs.

Product Features

- A unique collection of **600+** bioactive anti-virus compounds for HTS and HCS.
- Mainly target **HBV, HCV, HIV, HSV, Influenza Virus, Reverse Transcriptase**, etc.
- Bioactivity and safety have been confirmed by clinical trials and/or preclinical research. Some compounds have been approved by FDA.
- Detailed bioactivity information, including target, research areas, clinical information.
- High purity and quality validated by NMR and LC/MS.

Cat. No.: HY-L049

Antibacterial Compound Library

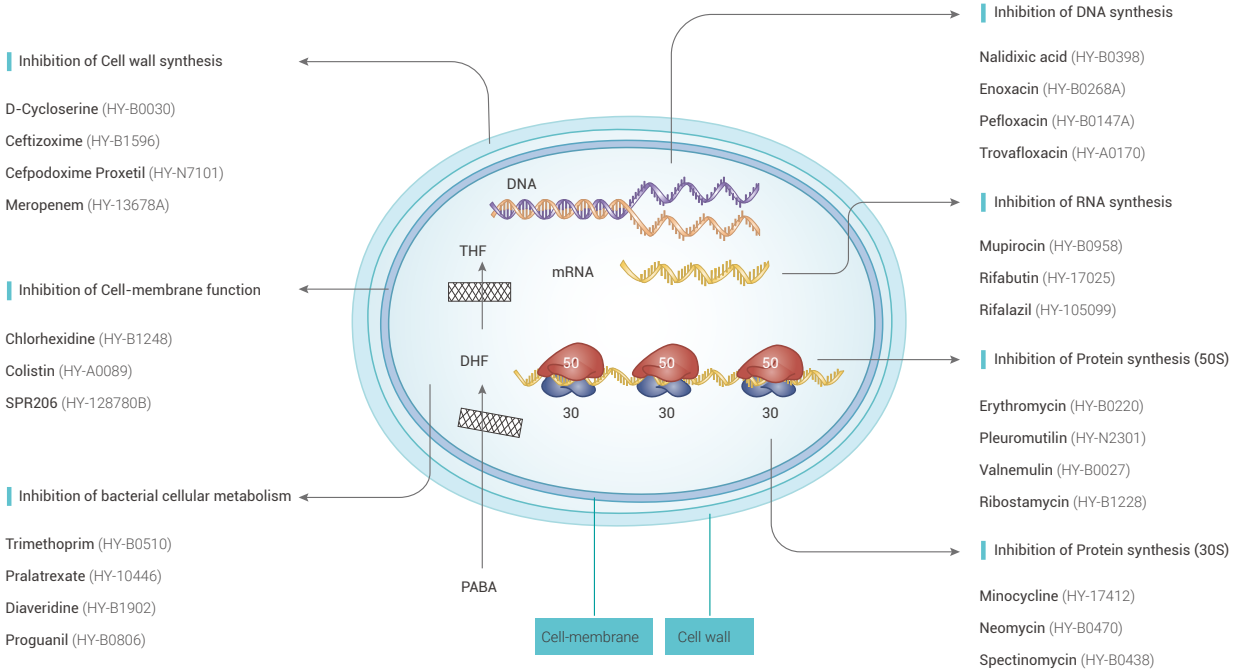
(96-/384-well plate)

Antibacterial agents are a group of materials that fight against pathogenic bacteria. Thus, by killing or reducing the metabolic activity of bacteria, their pathogenic effect in the biological environments will be minimized. The most widely used antibacterial agents exert their effects on bacterial cell wall synthesis, protein synthesis, DNA replication, and metabolic pathways. However, resistance to antimicrobial agents has become a major source of morbidity and mortality worldwide. The main mechanisms of resistance are limiting uptake of a drug, modification of a drug target, inactivation of a drug, and active efflux of a drug. Therefore, it is an urgent need to develop new drugs targeted at resistant organisms.

Product Features

- **800+** compounds have definite antibacterial activity and can be used for HTS and HCS.
- Act on various targets of bacteria, such as **cell wall, cell membranes, ribosomes, nucleic acids, bacterial cellular metabolism,** and **bacterial cellular enzymes**.
- Bioactivity and safety have been confirmed by clinical trials and/or preclinical research. Some compounds have been approved by FDA.
- High purity and quality validated by NMR and LC/MS.

Examples of Compounds with Different Mechanisms of Action



Classes of antibiotics/antibacterial agents and their modes of action on bacteria Scientific Research. Vol.6 No.5(2014).

Cat. No.: HY-L067

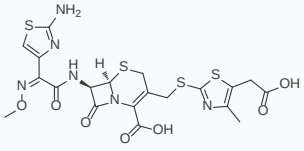
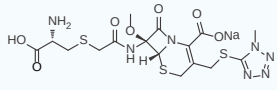
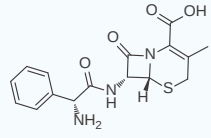
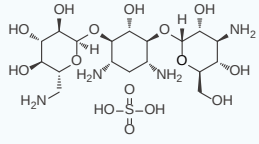
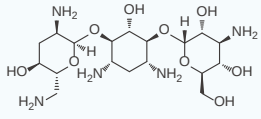
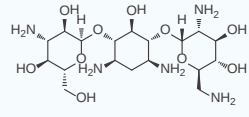
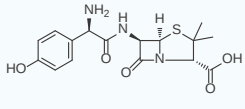
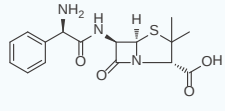
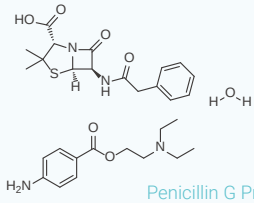
Antibiotics Library

(96-/384-well plate)

Product Features

- **500+ antibiotics** that can be used for HTS and HCS.
- Structurally diverse, including penicillins, cephalosporins, tetracyclines, macrolides, etc.
- Act on various targets on bacteria, such as **cell wall, cell membranes, ribosomes, nucleic acids, bacterial cellular metabolism** and **bacterial cellular enzymes.**
- Can be used in the study of new indications and the development of new anti-bacteria and anti-tumor drugs.
- Bioactivity and safety have been confirmed by clinical trials and/or preclinical research. Some compounds have been approved by FDA.
- High purity and quality validated by NMR and LC/MS.

Examples of Antibiotics

Cephalosporins	HY-108402  Cefodizime	HY-128932  Cefminox sodium	HY-B0200  Cephalexin
Aminoglycosides	HY-16566A  Kanamycin sulfate	HY-B0441  Tobramycin	HY-B1174  Bekanamycin
Penicillins	HY-B0467A  Amoxicillin	HY-B0522  Ampicillin	HY-N7120  Penicillin G Procaine

Cat. No.: HY-L048

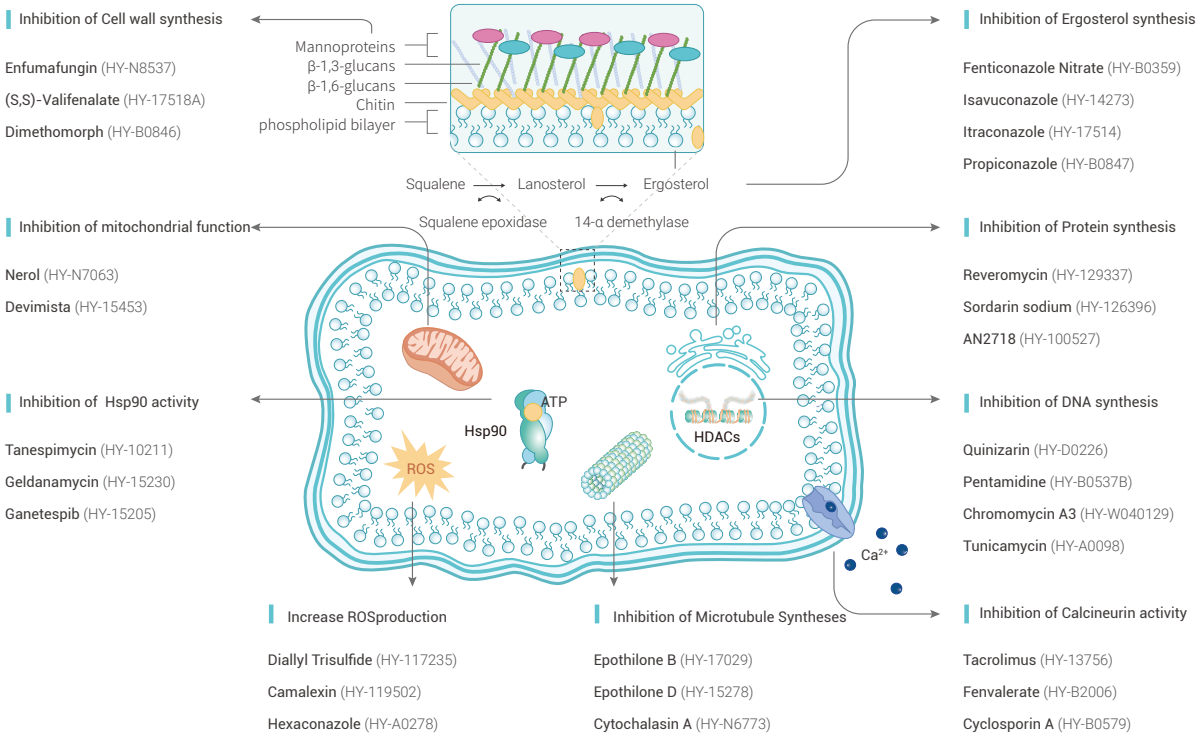
Antifungal Compound Library

(96-/384-well plate)

Product Features

- 250+ compounds have validated antifungal activity and can be used for HTS and HCS.
- Act on various targets of fungi, such as fungal RNA synthesis, cell wall and membrane components.
- The compound library can be used for the study of new indications and the development of new antifungal drugs.
- Bioactivity and safety have been confirmed by clinical trials and/or preclinical research. Some compounds have been approved by FDA.
- High purity and quality validated by NMR and LC/MS.

Examples of Antifungal Agents and Their Modes of Action on Fungi



Old and new targets as antifungal candidates
J Fungi (Basel). 2020 Oct 9;6(4):213.

Cat. No.: HY-L082

Antiparasitic Compound Library

(96-/384-well plate)

A parasite is an organism that lives on or in a host organism and gets its food from or at the expense of its host. Parasites of humans include protozoans, helminths, and ectoparasites. They are responsible for many diseases and are transmitted to their hosts most often through the ingestion of contaminated food, water or through the bite of an arthropod (e.g., a fly or tick), which can act as an intermediate host and as a vector. Parasitic diseases of humans are a major global health problem, especially in developing countries. Each year there are hundreds of millions of people infected with disease-causing parasites, particularly in tropical and subtropical regions of the world, resulting in an estimated one million deaths.

Product Features

- **300+** compounds that can be used for HTS and HCS.
- Compounds in this library have a variety of antiparasitic activities, including **anti-plasmodium, anti-leishmania, anti-filariasis,** and **anti-lymphatic filariasis,** etc.
- The compound library can be used for the study of new indications and the development of new antiparasitic drugs.
- Bioactivity and safety have been confirmed by clinical trials and/or preclinical research. Some compounds have been approved by FDA.
- High purity and quality validated by NMR and LC/MS.

Cat. No: HY-L073

Anti-Hepatitis C Virus Compound Library

(96-/384-well plate)

Globally, an estimated 71 million people have chronic hepatitis C virus infection. A significant number of those who are chronically infected will develop cirrhosis or liver cancer. To date, there is no vaccine against HCV. More recently, new therapeutic approaches that target essential components of the HCV life cycle have been developed, including direct-acting antiviral (DAA) that specifically block a viral enzyme or functional protein and host-targeted agents (HTA) that block interactions between host proteins and viral components that are essential to the viral life cycle. However, the genetic diversity of HCV viruses and the stage of liver disease (i.e., cirrhosis) are revealing themselves as obstacles for effective, pan-genotypic treatments. There still exists a need for the discovery and development of new HCV inhibitors.

Product Features:

- **200+** bioactive anti-hepatitis C virus compounds that can be used for HTS and HCS.
- Act on the main targets in HCV treatment, including **NS3, NS4A, NS5A,** RNA-dependent **RNA-polymerases, EGFR,** etc.
- Bioactivity and safety have been confirmed by clinical trials and/or preclinical research. Some compounds have been approved by FDA.
- High purity and quality validated by NMR and LC/MS.

Cat. No.: HY-L052

Anti-COVID-19 Compound Library

(96-/384-well plate)

COVID-19 poses a serious threat to people's health, and it is urgent to develop drugs to treat COVID-19 effectively. The screening of anti-COVID-19 drugs by using the clinical and approved compounds can greatly shorten the research and development cycle. Taking advantage of our virtual screening, MCE conducted virtual screening of approved compound library and clinical compound library based on the 3CL protease (PDB ID: 6LU7), Spike Glycoprotein (PDB ID: 6VSB), NSP15 (PDB ID: 6VWW), RDRP, PLPro and ACE2 structure. MCE designed a unique collection of compounds which may have anti-COVID-19 activity. The Library will be a powerful tool for screening new anti-COVID-19 drugs.

Product Features

- **1,500+** compounds are derived from virtual screening of approved compound library and clinical compound library based on the 3CL protease, Spike Glycoprotein and ACE2 structure.
- Bioactivity and safety have been confirmed by clinical trials and/or preclinical research.

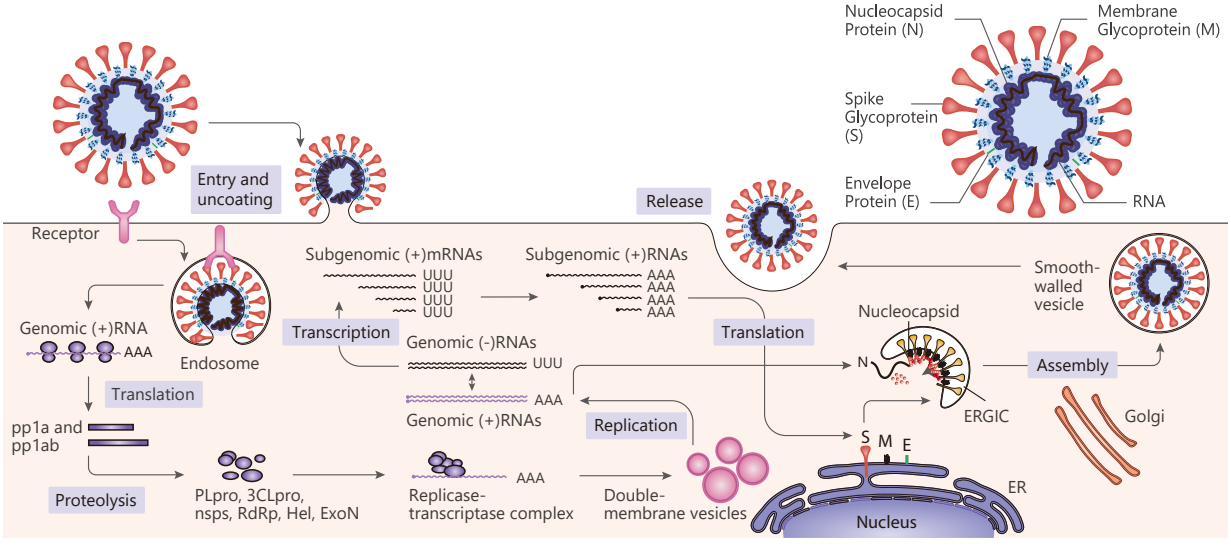
FAQ

— Do all the products in this library have definite anti-COVID-19 activity?

Compounds in this library were obtained by virtual screening based on the main targets of COVID-19. These compounds have potential anti-COVID-19 activity. However, there is no guarantee that all the products have anti-COVID-19 activity.

— Have these products entered the clinical trial in the anti-COVID-19 study?

The products in the library are in clinical trials or approved in other disease studies, but are not used in COVID-19 study. These products can be used to develop new indications for COVID-19 and speed up the development of anti-COVID-19 drugs based on the data and safety validation of these products in other diseases.

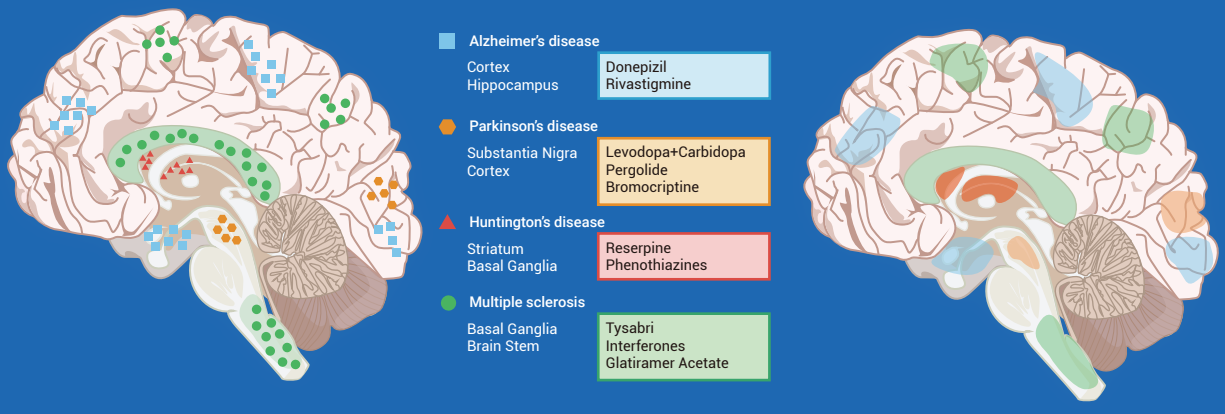


SARS-CoV and MERS-CoV structure and replication Nat Rev Microbiol. 2016 Aug;14(8):523-34.

Neurodegenerative Disease Series

Neurodegenerative diseases are characterized by progressive dysfunction and death of neurons and include a broad range of conditions, from Parkinson's (PD), Alzheimer's (AD), Huntington's disease (HD) to glaucoma. AD and PD mainly occur in middle-age and old people while HD, amyotrophic lateral sclerosis and spinal muscular atrophy may occur at any ages. At present, the cause of such diseases is not clear and there is no cure, and it is a serious threat to human health.

Recent research findings have led to a greater understanding of neurodegenerative diseases. Current studies on the pathogenesis of neurodegenerative diseases mainly include protein misfolding and aggregation, neuroinflammation, programmed cell death and aging, etc. These results not only provide useful information for elucidating the mechanism of these diseases, but also provide new ideas and targets for finding new drugs.



Major Neurodegenerative diseases, their associated regions, and current therapeutic interventions.[1]

- HY-L070 53
  Neuroprotective Compound Library
- HY-L069 53
  Anti-Alzheimer's Disease Compound Library
- HY-L085 53
  Anti-Parkinson's Disease Compound Library
- HY-L086 53
  Neurodegenerative Disease-Related Compound Library

Reference: [1] **Brain Sci.** 2018 Sep 15;8(9):177.

Product Name	Compound Number	Product Features
HY-L070 Neuroprotective Compound Library	700+	• Neuroprotection is an approach to prevent neurons from different pathological damages in neurodegenerative diseases.. • Act on some key targets in neuroprotective signaling pathways. • **Main targets**: Calcium channel, sodium channel, adenosine A1 receptor, PI3K, etc.
HY-L069 Anti-Alzheimer's Disease Compound Library	900+	• Several important mechanisms have been proposed to explain the underlying pathology of AD, such as Amyloid cascade hypothesis, Tau hypothesis and Cholinergic hypothesis, etc. • MCE carefully collects 900+ compounds that have potential anti- Alzheimer's disease activity. • **Main targets**: Amyloid-β, 5-HT Receptor, nAChR, etc.
HY-L085 Anti-Parkinson's Disease Compound Library	800+	• Compounds with anti-Parkinson's Disease activities or targeting the unique targets of PD which is a useful tool for exploring the mechanism of PD and discovering new drugs for PD. • **Main targets**: Dopamine Receptor, LRRK2, 5-HT Receptor, Monoamine Oxidase, nAChR, etc.
HY-L086 Neurodegenerative Disease-Related Compound Library	1,400+	• Compounds with anti-Neurodegenerative Diseases activities or targeting the unique targets of neurodegenerative diseases. • **Main targets**: Dopamine receptor, Amyloid β, COMT, LRRK2, nAChR, 5-HT receptor, Monoamine Oxidase, Histamine Receptor, etc.

Publications Citing Use of MCE Products in These Libraries

Neurosci Lett. 2021 Aug 10;759:136049. **Mol Cell Probes.** 2020 Apr;50:101498. **Genomics.** 2021 Jun 7;S0888-7543(21)00220-2.
Cell Metab. 2021 Oct 5;33(10):2040-2058.e10. **Cell Commun Signal.** 2020 May 4;18(1):70. **Oncogene.** 2019 Apr;38(14):2565-2579.

Other Disease Related Compound Libraries

(96-/384-well plate)

Product Name	Compound Number	Product Features
HY-L034 Anti-Aging Compound Library	2,700+	• Bioactive anti-aging compounds. • **Main targets**: Sirtuin, mTOR, IGF-1R, AMPK, p53, Telomerase, Mitophagy, Mitochondrial Metabolism, COX, Cytochrome P450, Oxidase, etc.
HY-L046 Anti-Cardiovascular Disease Compound Library	900+	• Bioactive anti-cardiovascular compounds for HTS and HCS. • **Main targets**: Metabolic enzyme, membrane transporter, ion channel, inflammation related signaling pathways, etc.
HY-L047 Endocrinology Compound Library	750+	• Bioactive compounds which can be used in the research of endocrine regulation. • **Main targets**: Thyroid hormone receptor, TSH receptor, GNRH receptor and adrenergic receptor related signaling pathways.
HY-L040 Diabetes Related Compound Library	500+	• Diabetes-related compounds. • **Main targets**: SGLT, PPAR, DPP-4, AMPK, Dipeptidyl Peptidase, Glucagon Receptor, etc.
HY-L087 Anti-Obesity Compound Library	400+	• Compounds that mainly target signaling pathway of controlling appetite, fatty acid metabolism and energy expenditure, etc. • **Main targets**: Fatty Acid Synthase (FASN), GLP-1R, Adrenergic receptor, MCHR1 (GPR24), Neuropeptide Y receptor, PARP, etc.

Virtual Screening Database

Library Name	Compound Quantity	Product Features
MCE Bioactive Compound Library	14,000+	A unique collection of 14000+ bioactive and structurally diverse compounds. Bioactivity and safety confirmed by preclinical research and clinical trials. Some have been approved by FDA.
MCE Fragment Library	16,000+	Latest release of Ro3 Fragment Library comprising over 16,000+ high-quality molecules. A useful tool for the fragment-based approach to drug discovery (FBDD).
Chemspace Lead-Like Compound Library	981,244	Chemspace Lead-Like Compound Library contains 981,244 in-Stock lead-like compounds with favorable physicochemical profiles and high Quantitative Estimation of Drug-likeness.
Chemspace Scaffold derived set	10,119	Composed of 10,119 compounds, which including 3,373 scaffolds, 3 compounds per each.
Chinese National Compound Library	1,398,968	~1.4 million compounds possessing diversified structures.
FCH Group Screening Library	2,244,487	FCH Group Screening Library contains about 2,244,487 lead-like compounds for biological screening.
InterBioScreen Synthetic Compounds Library	485,000	InterBioScreen Synthetic Compounds Library contains about 485,000 immediately available compounds.
Life Chemicals 50K Diversity Library	50,240	Life Chemicals 50K Diversity Library contains 50,240 diverse screening compounds.
Life Chemicals HTS Compound Collection	494,471	Life Chemicals HTS library is a unique collection contains 494,471 diverse screening compounds for the lead identification via high-throughput screening (HTS) and high content screening (HCS).
OTAVAchemicals Screening Collection	270,000	OTAVAchemicals Screening Collection contains about 270,000 re-supply compounds for prompt delivery.

Virtual Screening Database

Library Name	Compound Quantity	Product Features
Specs HTS Compounds Library	208,518	Specs HTS library is a unique collection contains 208,518 diverse screening compounds for the lead identification via high-throughput screening (HTS) and high content screening (HCS).
UORSY New Generation Screening Library	1,900,000	UORSY New Generation Screening Library contains about 1,900,000 compounds. The library is a revolutionary collection of lead-like molecules with outstanding structural quality and diversity—New Generation Screening Library (NGSL).
UORSY Screening Library	680,000	UORSY Screening Library contains about 680,000 compounds. The library has extensively developed a polymerization synthesis method that provides a highly diverse chemical structure.
Vitas-M Screening Compounds Library	1,400,000	Stock of synthetic small molecule organic compounds for biological screening and lead optimization. It is the best source to make "cherry pick" selection as per your criteria.

Customize Library

You can select

- √ Specific Compounds
- √ Quantities
- √ Plate Map
- √ Concentration
- √ Form (Solid or Solution)