

# Compound Screening Libraries

Optimized for Disease Mechanism Revealing & Drug Repurposing

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Bioactive Compound Library

FDA-Approved Drug Library

Anti-Cancer Compound Library

Kinase Inhibitor Library

Small Molecule Immuno-Oncology Compound Library

GPCR/G Protein Compound Library

Epigenetics Compound Library

Anti-Infection Compound Library

Anti-COVID-19 Compound Library

Clinical Compound Library

CNS-Penetrant Compound Library

Virtual Screening

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# Bioactive Compound Screening Libraries

## (96- or 384-well)



Our ready-to-use MedChemExpress (MCE) compound libraries consist of **over 10,000** small molecules with validated biological and pharmacological activities. They are available for **high-throughput screening (HTS)** and **high-content screening (HCS)**. Compound libraries are useful professional tools for drug discovery and new indication research.

- **Safety** and **effectiveness** have been confirmed by literature, patent reports and clinical research. Many products are **FDA-approved**.
- Focuses on hundreds of targets that are **key components** in the fields of GPCR, kinase, anti-cancer, epigenetics, stem cell biology, etc.
- Up-to-date with the latest **medical molecule** developments and offers access to our **exclusive Clinical Compound Library**.
- **Detailed biological and chemical information** are provided for every compound together with the LC/MS and NMR reports to ensure high quality.

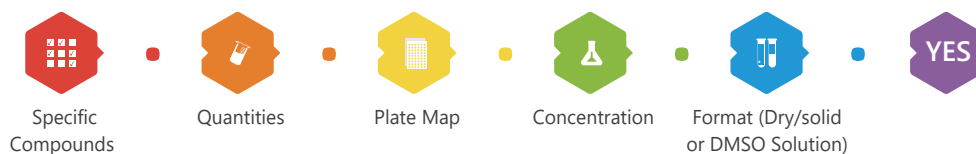
We offer **over 300 exclusive compounds worldwide** and track the latest scientific innovations to give our customers access to **the newest** small molecules. We are dedicated to providing **high-quality small molecules** to our customers around the world.



## Customize Your Library

MCE offers customized compound libraries based on your specific needs.

You can select compounds, format (powder/liquid), size and plate map depending on your requirements.





## Publications Citing Use of MCE Products

Nature. 2019 Dec;576(7786):274-280.

Nature. 2019 Nov;575(7784):683-687.

Nature. 2019 Nov;575(7782):375-379.

Nature. 2019 Oct;574(7777):264-267.

Nature. 2019 Jul;571(7763):127-131.

Nature. 2018 Nov;563(7729):131-136.

Nature. 2018 Oct;562(7728):600-604.

Science. 2020 Feb 14;367(6479):806-810.

Science. 2019 Jul 19;365(6450). pii: eaau6499.

Science. 2018 Sep 28;361(6409). pii: eaao4227.

Cell. 2020 Feb 20;180(4):645-654.e13.

Cell. 2019 Dec 12;179(7):1483-1498.e22.

Cell. 2019 Dec 12;179(7):1566-1581.e16.

Cell. 2019 Oct 31;179(4):864-879.e19.

Cell. 2019 Aug 22;178(5):1145-1158.e20.

Cell. 2019 Aug 22;178(5):1132-1144.e10.

Cell. 2019 Jul 25;178(3):585-599.e15.

Cell. 2019 Jul 11;178(2):330-345.e22.

Cell. 2019 Apr 4;177(2):370-383.e15.

Cell. 2019 Mar 7;176(6):1447-1460.e14.

Cell. 2019 Mar 6. pii: S0092-8674(19)30202-8.

Cell. 2019 Jan 24;176(3):505-519.e22.

Cell. 2019 Jan 24;176(3):636-648.e13.

Nat Nanotechnol. 2019 Oct;14(10):988-993.

Nat Biotechnol. 2019 Oct;37(10):1209-1216.

Nat Biotechnol. 2018 Feb;36(2):179-189.

... See more citations on [www.MedChemExpress.com](http://www.MedChemExpress.com)





## MCE Screening Library Partners





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# Bioactive Compound Library

Cat. No.: HY-L001

Product Name	Cat. No.	Compounds	Size (Pre-dissolved in DMSO/Solid)
Bioactive Compound Library	HY-L001	7,000+	30 $\mu$ L/well, 50 $\mu$ L/well, 100 $\mu$ L/well, 250 $\mu$ L/well (10 mM solution)

- A unique collection of **7,000+** bioactive compounds including natural products, enzyme inhibitors, receptor ligands, and drugs for **high throughput screening (HTS)** and **high content screening (HCS)**.
- Bioactivity and safety confirmed by preclinical research and clinical trials. Some have been approved by FDA.
- Widely used in the research focus areas such as **Cancer, Stem Cell, Neuronal Signaling, Immunity**, and more.
- Structurally diverse, medicinally active, and cell permeable.
- More detailed compound information with structure, IC<sub>50</sub>, and other chemical & biological data.
- NMR and HPLC validated to ensure high purity and quality.
- All compounds are in stock and continuously updated.

## Targets Included in Bioactive Compound Library:

5-HT Receptor	ACE	Adenosine Receptor	AChE	Adrenergic Receptor	Akt	Androgen Receptor
Angiotensin Receptor	ALK	Antibacterial	Antifolate	Antifungal	Apoptosis	Antiparasitic
ATM/ATR	Aurora Kinase	Bcl-2 Family	Bcr-Abl	Calcium Channel	Casein Kinase	Cannabinoid Receptor
CDK	c-Kit	c-Met/HGFR	COX	Cytochrome P450	CXCR	DNA Alkylator/Crosslinker
DNA/RNA Synthesis	DPP4	Dopamine Receptor	EGFR	Epigenetic Reader Domain	ERK	Estrogen Receptor/ERR
FGFR	FLT3	GABA Receptor	GSK-3	Glucocorticoid Receptor	HCV	HDAC
HIF/HIF Prolyl-Hydroxylase	HIV	Histamine Receptor	HSP	Histone Methyltransferase	HSV	IGF-1R
IKK	JAK	LRRK2	mAChR	MDM-2/p53	MEK	mGluR
Microtubule/Tubulin	mTOR	nAChR	NF- $\kappa$ B	NMDA Receptor	OX Receptor	Opioid Receptor
P2X Receptor	p38 MAPK	p97	PAI-1	PAK	Parasite	PARP
PD-1/PD-L1	PDGFR	PDHK	PDK-1	PGE Synthase	PERK	P-glycoprotein
Phosphatase	PDE	Phospholipase	PI3K	PI4K	Pim	PKA
PKC	PKD	Polo-like Kinase (PLK)	Porcupine	Potassium Channel	PPAR	Progesterone Receptor
Prostaglandin Receptor	Proteasome	PAR	Proton Pump	Pyruvate Kinase	PTEN	Potassium Channel
RAD51	Raf	RAR/RXR	Ras	Ribosomal S6 Kinase (RSK)	RIP Kinase	ROCK
Reverse Transcriptase	ROR	ROS	RSV	Ser/Thr Protease	SGK	Serotonin Transporter
Sigma Receptor	SGLT	Sirtuin	Smo	Sodium Channel	SPHK	Src
STING	STAT	Syk	Telomerase			
TGF-beta/Smad	Thrombin	TGF- $\beta$ Receptor	TAM Receptor			
Thyroid Hormone Receptor	TOPK	Toll-like Receptor (TLR)	TNF Receptor			
Tryptophan Hydroxylase	TRP Channel	Tyrosinase	Trk Receptor			
Topoisomerase	ULK	Urotensin Receptor	URAT1			
Vasopressin Receptor	VEGFR	Wee1	Wnt			
Xanthine Oxidase	$\beta$ -catenin	$\gamma$ -secretase	...			

### Customize Library

#### You can select:

- ✓ Specific Compounds
- ✓ Quantities
- ✓ Plate Map
- ✓ Concentration
- ✓ Format (Dry/Solid or DMSO Solution)

## Bioactive Compound Library Plus

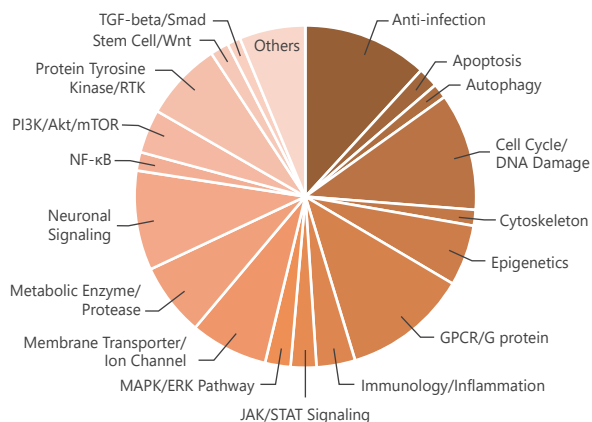
Cat. No.: HY-L001P

Product Name	Cat. No.	Compounds	Size (Pre-dissolved in DMSO/Solid)
Bioactive Compound Library Plus	HY-L001P	9,000+	30 µL/well, 50 µL/well, 100 µL/well, 250 µL/well (10 mM solution)

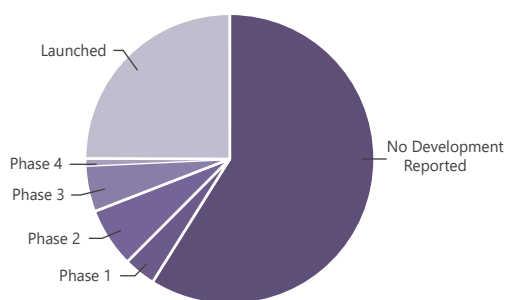
- A unique collection of **9,000+** bioactive compounds including natural products, enzyme inhibitors, receptor ligands, and drugs for **high throughput screening (HTS)** and **high content screening (HCS)**.
- The library consists of HY-L001 (Part A), compounds with low solubility or stability (Part B) and novel or rare compounds (Part C).
- Bioactivity and safety confirmed by preclinical research and clinical trials. Some have been approved by **FDA**.
- Widely used in the research focus areas such as **Cancer, Stem Cell, Neuronal Signaling, Immunity**, and more.
- Structurally diverse, medicinally active, and cell permeable.
- More detailed compound information with structure, IC<sub>50</sub>, and other chemical & biological data.
- NMR and HPLC validated to ensure high purity and quality.

	Part A	Part B	Part C
Number	7,000+	800+	800+
Feature	General compounds (HY-L001)	Compounds with low solubility or stability	Novel, rare or exclusive compounds
Package	Solution (10 mM) or solid (1 mg)	Only solid (1 mg)	Only solid (1 mg)

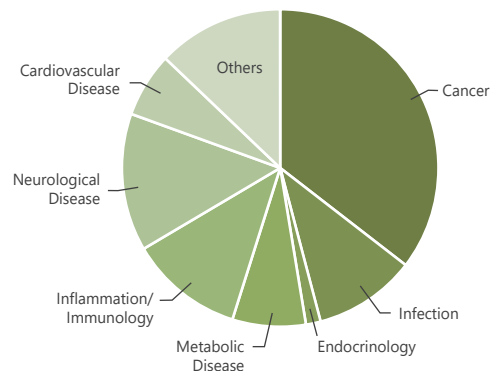
Targeted Pathways of Bioactive Compounds



Clinical Phase for Bioactive Compounds



Targeted Research Areas of Bioactive Compounds



### Publications Citing Use of MCE Bioactive Library Compounds:

**Nature**. 2018 Nov;563(7729):131-136.

**Nature**. 2018 Oct;562(7728):600-604.

**Science**. 2018 Sep 28;361(6409). pii: eaao4227.

**Cell**. 2019 Mar 7;176(6):1447-1460.e14.

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## Fragment Library

Cat. No.: HY-L032

Product Name	Cat. No.	Compounds	Size (Pre-dissolved in DMSO/Solid)
Fragment Library	HY-L032	8,000+	50 µL/well, 100 µL/well (10 mM solution)

- A unique collection of **8,000+** fragment compounds for traditional lead identification via **high-throughput screening (HTS)**.
- The compounds follow the **Rule of Three**.
- A useful tool for the **fragment-based approach to drug discovery (FBDD)**.
- More detailed compound information with structure, Molecular Weight, cLogP, H-donor and H-acceptor number.
- NMR and HPLC validated ensure high purity.
- All compounds are in stock and continuously updated.

Parameter	Range	Average Value
Molecular Weight	≤300	179.20
cLogP	≤3.0	1.2944
H-donors	≤3.0	2.20
H-acceptors	≤3.0	0.81

### Publications Citing Use of MCE Compound Screening Libraries:

Nat Med. 2017 Apr 7;23(4):405-408.

Nat Commun. 2018 Apr 26;9(1):1677.

Cell Syst. 2018 Apr 25;6(4):424-443.e7.

Cell Rep. 2017 Jul 25;20(4):999-1015.

J Med Chem. 2018 Jan 11;61(1):360-371.

ACS Chem Biol. 2016 Dec 16;11(12):3400-3411.

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### Customize Library

#### You can select:

- ✓ Specific Compounds
- ✓ Quantities
- ✓ Plate Map
- ✓ Concentration
- ✓ Format (Dry/Solid or DMSO Solution)



## FDA-Approved Drug Library

Product Name	Cat. No.	Compounds	Size (Pre-dissolved in DMSO/Solid)
FDA-Approved Drug Library	HY-L022	1,800+	30 µL/well, 50 µL/well, 100 µL/well, 250 µL/well (10 mM solution)
FDA-Approved Drug Library Plus	HY-L022P	2,000+	30 µL/well, 50 µL/well, 100 µL/well, 250 µL/well (10 mM solution)

- A unique collection of marketed drugs for **high throughput screening (HTS)** and **high content screening (HCS)**.
- Used in the research of **oncology, cardiology, anti-inflammatory, immunology, dermatology, endocrinology, neurology**, and more.
- A useful tool for **researching new targets of marketed old drugs**.
- All compounds have been approved by the **FDA** or **EMA**.
- Structurally diverse, bioactive, and cell permeable.
- More detailed compound information with structure, IC<sub>50</sub>, and brief introduction.
- NMR and HPLC validated ensure high purity.
- All compounds are in stock and continuously updated.

### Targets Included in FDA-Approved Drug Library:

5 alpha Reductase	5-HT Receptor	ACE	AChE	Adenosine Receptor	ALK	Adrenergic Receptor
Androgen Receptor	Angiotensin Receptor	Antibacterial	Antifolate	Antifungal	Antiparasitic	Autophagy
Bcr-Abl	Calcium Channel	CaSR	Carbonic Anhydrase	c-Kit	c-Met/HGFR	Cytochrome P450
CXCR	DNA alkylator	DPP4	DNA/RNA Synthesis	Dopamine Receptor	EGFR	Endothelin Receptor
Estrogen Receptor	Factor Xa	GABA Receptor	Glucocorticoid Receptor	HBV	HCN Channel	HCV
HDAC	Histamine Receptor	HIV	HMG-CoA Reductase	HSV	Influenza Virus	JAK
Leukotriene Receptor	mAChR	mGluR	Microtubule/Tubulin	Monoamine Oxidase	nAChR	Neurokinin Receptor
NMDA Receptor	NNRTIs	NRTIs	Opioid Receptor	P2Y Receptor	PDE	PDGFR
PGE synthase	Potassium Channel	PKC	Progesterone Receptor	PPAR	Proteasome	Proton Pump
Raf	RAR/RXR	Ras	Sodium Channel	SGLT	Src	SSRIs
STAT	Thrombin	TNF-alpha	Topoisomerase	Vasopressin Receptor	VEGFR	Xanthine Oxidase ...

### Publications Citing Use of MCE FDA-Approved Library Drugs:

**Nature.** 2018 Nov;563(7729):131-136.

**Nature.** 2018 Aug;560(7719):499-503.

**Nat Med.** 2018 Aug;24(8):1143-1150.

**Nat Commun.** 2018 Dec 10;9(1):5272.

**Nat Commun.** 2018 Apr 26;9(1):1677.

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## FDA-Approved Drug Library Mini

Cat. No.: HY-L022M

Product Name	Cat. No.	Compounds	Size (Pre-dissolved in DMSO)
FDA-Approved Drug Library Mini	HY-L022M	1,800+	10 $\mu$ L/well (10 mM solution)

- A unique collection of 1,800+ marketed drugs for high throughput screening (HTS) and high content screening (HCS).
- Used in the research of oncology, cardiology, anti-inflammatory, immunology, dermatology, endocrinology, neurology, and more.
- A useful tool for researching new targets of marketed old drugs.
- Easily peelable foil seal makes the screening process easier and faster.
- Lower price, more compounds.
- Avoid multiple and uneven dispensing.
- Reduce risks of product cross-contamination.
- Avoid reduced activity due to long-term storage.

FDA-Approved Drug Library Mini

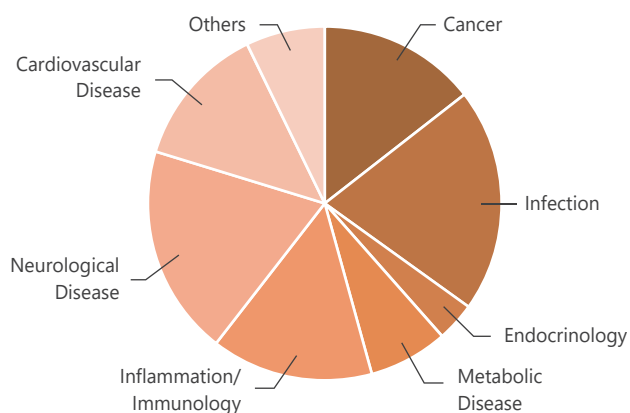


FDA-Approved Drug Library (Cat. No.: HY-L022)



Size	10 $\mu$ L in DMSO	30, 50, 100, and 250 $\mu$ L in DMSO
Package	96-well microplate with peelable foil seal	96-Well Format Sample Storage Tube With Screw Cap
Delivery Date	Within three days	About one month
Price Per Set	Low	High
Preparation For Use	Tear off the seal film on the microplate	If there is no robot, each tube needs to be manually opened

Principle Research Areas of FDA-Approved Drug Library



### Customize Library

#### You can select:

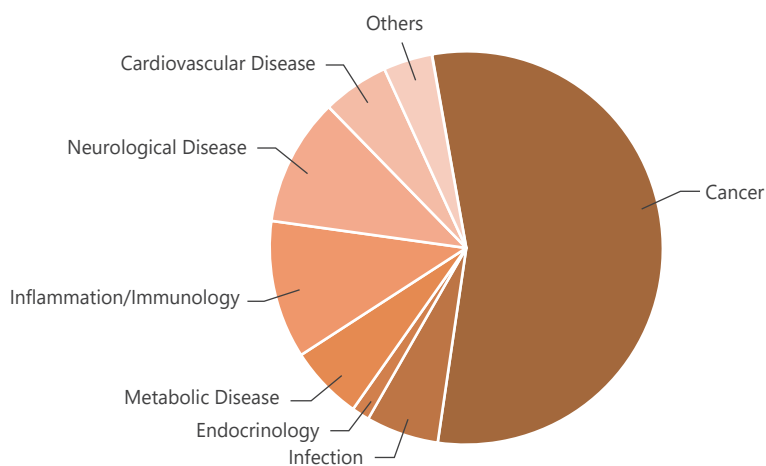
- ✓ Specific Compounds
- ✓ Quantities
- ✓ Plate Map
- ✓ Concentration
- ✓ Format (Dry/Solid or DMSO Solution)

## Clinical Compound Library

Product Name	Cat. No.	Compounds	Size (Pre-dissolved in DMSO/Solid)
Clinical Compound Library	HY-L026	1,100+	30 µL/well, 50 µL/well, 100 µL/well, 250 µL/well (10 mM solution)
Clinical Compound Library Plus	HY-L026P	1,300+	30 µL/well, 50 µL/well, 100 µL/well, 250 µL/well (10 mM solution)

- A unique collection of clinical compounds for **high throughput screening (HTS)** and **high content screening (HCS)**.
- Research areas include **anticancer**, **anti-infection**, **anti inflammation**, **nervous disease**, and more.
- A useful tool for drug repurposing, the application of an existing therapeutic to a new disease indication.
- **Currently in clinical stage**, some are withdrawn or terminated.
- Structurally diverse, medicinally active, and cell permeable.
- Detailed compound information with structure, IC<sub>50</sub>, and brief introduction.
- Validated NMR and HPLC to ensure high purity and quality.
- All compounds are in stock and continuously updated.

Principle Research Areas of Clinical Compound Library



### 📖 Publications Citing Use of MCE Clinical Library Compounds:

**Nature.** 2018 Aug;560(7719):499-503.

**Nature.** 2018 Jun;558(7711):540-546.

**Science.** 2017 Dec 1;358(6367).

**Nat Med.** 2018 Nov;24(11):1752-1761.

**Cell.** 2019 Mar 7;176(6):1447-1460.e14.

**Cell.** 2019 Jan 24;176(3):636-648.e13.

**Cell.** 2018 Nov 1;175(4):984-997.e24.

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# Anti-Cancer Compound Library

Cat. No.: HY-L025

Product Name	Cat. No.	Compounds	Size (Pre-dissolved in DMSO/Solid)
Anti-Cancer Compound Library	HY-L025	3,200+	30 µL/well, 50 µL/well, 100 µL/well, 250 µL/well (10 mM solution)

- A unique collection of 3,200+ bioactive anti-cancer compounds for **high throughput screening (HTS)** and **high content screening (HCS)**.
- Targets include **kinases, cell cycle key components, tumorigenesis related signaling pathways, popular targets in epigenetic studies**, and more.
- A useful tool for the **discovery of anti-cancer drugs**.
- Bioactivity and safety confirmed by preclinical research and clinical trials. Some have been approved by FDA.
- Structurally diverse, medically active, and cell permeable.
- Detailed compound information with structure, IC<sub>50</sub>, and brief introduction.
- Validated NMR and HPLC to ensure high purity and quality.
- All compounds are in stock and continuously updated.

## Targets Included in Anti-Cancer Compound Library:

5 alpha Reductase	Ack1	ADC Cytotoxin	Akt	Aldose Reductase	ALK	AMPK
Antibacterial	Androgen Receptor	Antifolate	ATM/ATR	Apoptosis	Aurora Kinase	Autophagy
Axl	Bcl-2 Family	Bcr-Abl	BCRP	Btk	Casein Kinase	Cannabinoid Receptor
Caspase	CDK	c-Fms	Checkpoint Kinase (Chk)	c-Kit	c-Met/HGFR	CXCR
Deubiquitinase	DNA alkylator	DNA-PK	DNA Methyltransferase	E1/E2/E3 Enzyme	EGFR	Epigenetic Reader Domain
ERK	Estrogen Receptor	FAK	Farnesyl Transferase	FGFR	FLT3	GSK-3
HDAC	Hedgehog	Hexokinase	HIF/HIF Prolyl-Hydroxylase	Histone Demethylase	HSP	Histone Methyltransferase
IAP	IGF-1R	IKK	IDO	Insulin Receptor	Integrin	IDH
JAK	JNK	Keap1-Nrf2	KSP	MDM-2/p53	MEK	Microtubule/Tubulin
MMP	mTOR	Myosin	Nampt	NF-κB	P2X Receptor	Nucleoside antimetabolite
p38 MAPK	p97	PAK	PARP	PDGFR	PDK-1	PERK
P-glycoprotein	Phospholipase	PI3K	Pim	PKC	PKD	Polo-like Kinase (PLK)
PPAR	Proteasome	Raf	RAR/RXR	Ras	ROCK	Ribosomal S6 Kinase
ROR	Sigma Receptor	Sirtuin	Smo	Src	STAT	Syk
TNF-alpha	TGF-β Receptor	TLR	Topoisomerase	Trk Receptor	VEGFR	Wnt/β-catenin ...

## Publications Citing Use of MCE Anti-Cancer Library Compounds:

**Nature.** 2018 Nov;563(7729):131-136.

**Science.** 2018 Sep 28;361(6409).

**Nat Med.** 2019 Feb;25(2):292-300.

**Cell.** 2019 Jan 24;176(3):505-519.e22.

**Cell.** 2018 Oct 4;175(2):442-457.e23.

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## Customize Library

### You can select:

- ✓ Specific Compounds
- ✓ Quantities
- ✓ Plate Map
- ✓ Concentration
- ✓ Format (Dry/Solid or DMSO Solution)

## Small Molecule Immuno-Oncology Compound Library

Cat. No.: HY-L031

Product Name	Cat. No.	Compounds	Size (Pre-dissolved in DMSO/Solid)
Small Molecule Immuno-Oncology Compound Library	HY-L031	150+	30 µL/well, 50 µL/well, 100 µL/well, 250 µL/well (10 mM solution)

- A unique collection of 150+ bioactive tumor immunology compounds for **high throughput screening (HTS)** and **high content screening (HCS)**.
- A useful tool for **cancer research** by activation of an antitumor immune response.
- Small molecule compounds targeting **PD1/PD-L1, ROR, CCR, CXCR, Sting, IDO, TLR**, etc.
- Bioactivity and safety confirmed by preclinical research and clinical trials, some have been approved by FDA.
- Structurally diverse, medicinally active, and cell permeable.
- More detailed compound information with structure, IC<sub>50</sub>, and other chemical & biological data.
- NMR and HPLC validated to ensure high purity and quality.
- All compounds are in stock and continuously updated.

### Publications Citing Use of MCE Small Molecule Immuno-Oncology Library Compounds:

**Gastroenterology**. 2018 May;154(6):1822-1835.e2.

**Cell Res**. 2018 Mar;28(3):323-335.

**Circ Res**. 2018 May 25;122(11):1532-1544.

**J Allergy Clin Immunol**. 2018 Jun;141(6):2286-2289.e5.

**Nat Commun**. 2019 Mar 4;10(1):1015.

**Nucleic Acids Res**. 2018 Apr 20;46(7):3284-3297.

**Autophagy**. 2019 Mar 25:1-17.

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## Anti-Infection Compound Library

Cat. No.: HY-L002

Product Name	Cat. No.	Compounds	Size (Pre-dissolved in DMSO/Solid)
Anti-Infection Compound Library	HY-L002	900+	30 $\mu$ L/well, 50 $\mu$ L/well, 100 $\mu$ L/well, 250 $\mu$ L/well (10 mM solution)

- A unique collection of **900+** bioactive anti-infection compounds for **high throughput screening (HTS)** and **high content screening (HCS)**.
- Targets such as **Bacteria, Fungi, Parasite, CMV, HIV, SARS-CoV, Influenza Virus**, etc.
- Bioactivity and safety confirmed by preclinical research and clinical trials, some have been approved by FDA.
- A useful tool to study infectious diseases or develop new anti-infection drugs.
- Structurally diverse, medicinally active, and cell permeable.
- More detailed compound information with structure, IC<sub>50</sub>, and other chemical & biological data.
- NMR and HPLC validated to ensure high purity and quality.
- All compounds are in stock and continuously updated.

### Targets Included in Anti-Infection Compound Library:

Antibacterial	Antifungal	Antiparasitic	CMV	Filovirus
HBV	HCV	HIV	HSV	Influenza Virus
NNRTIs	NRTIs	Rhinovirus (HRV)	RSV	SARS-CoV ...

### Publications Citing Use of MCE Anti-Infection Library Compounds:

*Science*. 2017 Dec 1;358(6367).

*Nat Methods*. 2018 Jul;15(7):519-522.

*Cell Metab*. 2018 Oct. DOI:10.2139/ssrn.3255557.

*Immunity*. 2018 Jul 17;49(1):80-92.e7.

*Sci Transl Med*. 2018 Jul 18;10(450).

*Circ Res*. 2018 May 25;122(11):1532-1544.

*Blood*. 2018 Jul 19;132(3):307-320.

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### Customize Library

#### You can select:

- ✓ Specific Compounds
- ✓ Quantities
- ✓ Plate Map
- ✓ Concentration
- ✓ Format (Dry/Solid or DMSO Solution)

## Anti-Virus Compound Library

Cat. No.: HY-L027

Product Name	Cat. No.	Compounds	Size (Pre-dissolved in DMSO/Solid)
Anti-Virus Compound Library	HY-L027	300+	30 µL/well, 50 µL/well, 100 µL/well, 250 µL/well (10 mM solution)

- A unique collection of 300+ bioactive anti-virus compounds for **high throughput screening (HTS)** and **high content screening (HCS)**.
- Targets include **HBV, HCV, HIV, HSV, Influenza Virus, Reverse Transcriptase**, etc.
- A useful tool for the discovery of anti-virus drugs.
- Bioactivity and safety confirmed by preclinical research and clinical trials. Some have been approved by FDA.
- Structurally diverse, medicinally active, and cell permeable.
- Detailed compound information with structure, IC<sub>50</sub>, and brief introduction.
- Validated NMR and HPLC to ensure high purity and quality.
- All compounds are in stock and continuously updated.

### Publications Citing Use of MCE Anti-Virus Library Compounds:

**Nat Immunol.** 2017 Dec;18(12):1299-1309.

**Sci Transl Med.** 2018 Jul 18;10(450).

**Hepatology.** 2019 May;69(5):1861-1872.

**Nat Commun.** 2018 Apr 26;9(1):1677.

**Nucleic Acids Res.** 2018 Jan 25;46(2):956-971.

**Nucleic Acids Res.** 2017 May 5;45(8):4743-4755.

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## Anti-COVID-19 Compound Library

Cat. No.: HY-L052

Product Name	Cat. No.	Compounds	Size (Pre-dissolved in DMSO/Solid)
Anti-COVID-19 Compound Library	HY-L052	1,001	30 µL/well, 50 µL/well, 100 µL/well, 250 µL/well (10 mM solution)

COVID-19 poses a serious threat to people's health, and it is urgent to develop drugs to treat COVID-19 quickly. The screening of anti-COVID-19 drugs by using the clinical and approved compounds can greatly shorten the research and development cycle. In addition, the virtual screening technology can effectively narrow the scope of screening and improve the screening efficiency in the pre-screening of new drugs.

Taking advantage of our virtual screening, we conduct virtual screening of approved compound library and clinical compound library based on the **3CL protease (Mpro, PDB ID: 6LU7)**, **Spike Glycoprotein** and **ACE2 (Angiotensin Converting Enzyme2)** structure. We design a unique collection of 1,001 compounds which may have anti-COVID-19 activity. Anti-COVID-19 Compound Library will be a powerful tool for screening new anti-COVID-19 activity drugs.

## CNS-Penetrant Compound Library

Cat. No.: HY-L028

Product Name	Cat. No.	Compounds	Size (Pre-dissolved in DMSO/Solid)
CNS-Penetrant Compound Library	HY-L028	400+	30 µL/well, 50 µL/well, 100 µL/well, 250 µL/well (10 mM solution)

- A unique collection of **400+** bioactive CNS-penetrant compounds for **high throughput screening (HTS)** and **high content screening (HCS)**.
- Targets such as **Kinases**, **GPCR** and **Ion Channels**, and more.
- A useful tool for the discovery of drugs used for **brain diseases**, such as brain tumors, mental disorders, and neurodegenerative diseases.
- Bioactivity and safety confirmed by preclinical research and clinical trials. Some inhibitors have been approved by FDA.
- Structurally diverse, medicinally active, CNS-penetrant and cell permeable.
- More detailed compound information with structure, IC50, and brief introduction.
- NMR and HPLC validated to ensure high purity and quality.
- All compounds are in stock and continuously updated.

### Targets Included in CNS-Penetrant Compound Library:

5-HT Receptor	AChE	ADC Cytotoxin	Adenosine Receptor	Adrenergic Receptor
Amyloid-β	Antibacterial	Antifolate	Antifungal	Antiparasitic
Bcr-Abl	Calcium Channel	Carbonic Anhydrase	CDK	c-Kit
COMT	COX	DNA Alkylator/Crosslinker	DNA/RNA Synthesis	Dopamine Receptor
EGFR	Estrogen Receptor/ERR	GABA Receptor	Histamine Receptor	HIV
HIV Protease	HMG-CoA Reductase	HSV	Influenza Virus	Melatonin Receptor
mGluR	mTOR	nAChR	Neurokinin Receptor	NMDA Receptor
NRTIs	Nucleoside Antimetabolite	p38 MAPK	PDE	PDGFR
PGE Synthase	Raf	Sodium Channel	Src	VEGFR ...

### Publications Citing Use of MCE CNS-Penetrant Library Compounds:

**Nature.** 2018 Nov;563(7729):131-136.

**Cell.** 2019 Jan 24;176(3):505-519.e22.

**Cell.** 2018 Sep 20;175(1):186-199.e19.

**Cell.** 2018 Sep 20;175(1):171-185.e25.

**Cell.** 2018 Aug 9;174(4):843-855.e19.

**Cancer Discov.** 2018 Mar;8(3):354-369.

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### Customize Library

#### You can select:

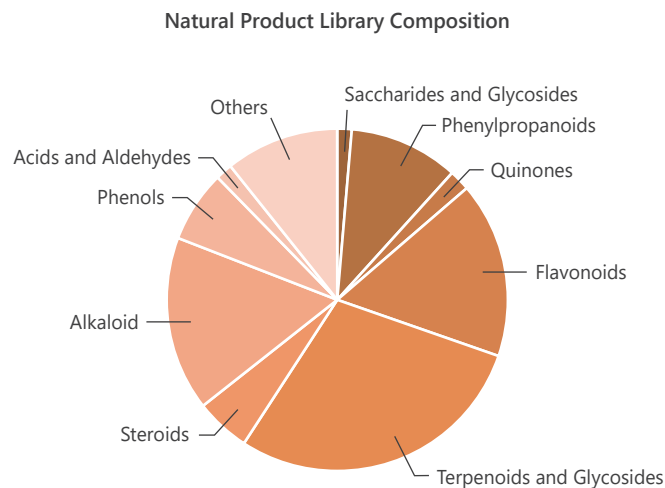
- ✓ Specific Compounds
- ✓ Quantities
- ✓ Plate Map
- ✓ Concentration
- ✓ Format (Dry/Solid or DMSO Solution)



## Natural Product Library

Product Name	Cat. No.	Compounds	Size (Pre-dissolved in DMSO/Solid)
Natural Product Library	HY-L021	1,400+	30 µL/well, 50 µL/well, 100 µL/well, 250 µL/well (10 mM solution)
Natural Product Library Plus	HY-L021P	2,000+	30 µL/well, 50 µL/well, 100 µL/well, 250 µL/well (10 mM solution)

- A unique collection of natural products for high throughput screening (HTS) and high content screening (HCS).
- The compounds in the library contain **Saccharides and Glycosides, Phenylpropanoids, Quinones, Flavonoids, Terpenoids and Glycosides, Steroids, Alkaloid, Phenols, Acids and Aldehydes.**
- A useful tool for drug discovery as an important source of lead compounds.
- Bioactivity and safety confirmed by preclinical research and clinical trials. Some compounds have been approved by FDA.
- Structurally diverse, bioactive, and cell permeable.
- More detailed compound information with structure, IC<sub>50</sub>, and brief introduction.
- NMR and HPLC validated ensure high purity.
- All compounds are in stock and continuously updated.



### Publications Citing Use of MCE Natural Library Products:

*Science*. 2017 Dec 1;358(6367).

*Nat Med*. 2019 Feb;25(2):337-349.

*Cell*. 2018 Oct 4;175(2):442-457.e23.

*Immunity*. 2018 Jul 17;49(1):80-92.e7.

*Cell Res*. 2019 Mar;29(3):193-205.

*Circ Res*. 2018 May 25;122(11):1532-1544.

*Blood*. 2018 Jul 19;132(3):307-320.

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## Toxins for Antibody-Drug Conjugate Research Library

Cat. No.: HY-L023

Product Name	Cat. No.	Compounds	Size (Solid)
Toxins for Antibody-Drug Conjugate Research Library	HY-L023	30+	1 mg

- A unique collection of 30+ ADC cytotoxins for targeted therapy research.
- Used to develop new antibody-drug conjugates targeting cancer.
- Bioactivity and safety confirmed by preclinical research and clinical trials.
- Structurally diverse, medicinally active, and cell permeable.
- More detailed compound information with structure, IC<sub>50</sub>, and brief introduction.
- NMR and HPLC validated to ensure high purity and quality.
- All compounds are in stock and continuously updated.

### Publications Citing Use of MCE Antibody-Drug Conjugate Research Library Toxins:

Nat Med. 2017 Apr 7;23(4):405-408.

Nat Microbiol. 2018 Nov;3(11):1266-1273.

Nat Commun. 2018 Oct 8;9(1):4139.

Nat Commun. 2018 Apr 30;9(1):1726.

Dev Cell. 2018 Sep 24;46(6):681-695.e5.

J Control Release. 2018 May 10;277:23-34.

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### Customize Library

#### You can select:

- ✓ Specific Compounds
- ✓ Quantities
- ✓ Plate Map
- ✓ Concentration
- ✓ Format (Dry/Solid or DMSO Solution)

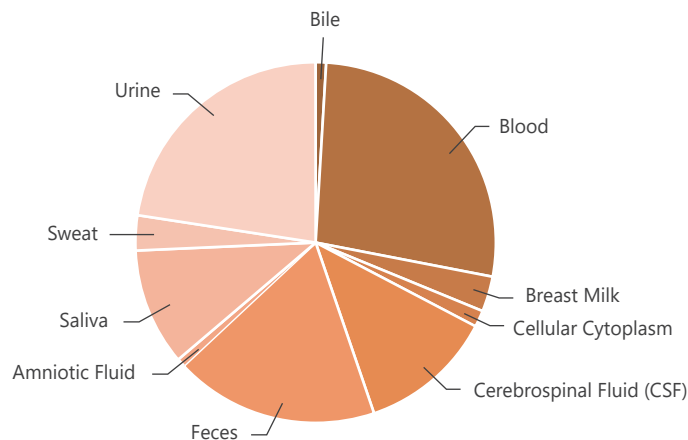
## Human Endogenous Metabolite Compound Library

Cat. No.: HY-L030

Product Name	Cat. No.	Compounds	Size (Pre-dissolved in DMSO/Solid)
Human Endogenous Metabolite Compound Library	HY-L030	400+	30 µL/well, 50 µL/well, 100 µL/well, 250 µL/well (10 mM solution)

- A unique collection of **400+** human endogenous metabolites for **high throughput screening (HTS)** and **high content screening (HCS)**.
- The compounds derived from human issues with better bioavailability.
- A useful tool for **metabonomics** and **metabolism-related drug discovery**.
- Bioactivity and safety confirmed by preclinical research and clinical trials. Some compounds have been approved by FDA.
- Structurally diverse, bioactive, and cell permeable.
- More detailed compound information with structure, IC<sub>50</sub>, and brief introduction.
- NMR and HPLC validated ensure high purity.
- All compounds are in stock and continuously updated.

Species of Compounds in Human Endogenous Metabolite Compound Library



### 📖 Publications Citing Use of MCE Human Endogenous Metabolite Library Compounds:

Cell Res. 2019 Mar;29(3):193-205.

Autophagy. 2019 Mar 25;1-17.

PLoS Biol. 2018 Oct 18;16(10):e2006483.

ACS Appl Mater Interfaces. 2019 Mar 20;11(11):10554-10558.

J Autoimmun. 2019 May;99:39-47.

Br J Pharmacol. 2019 Mar 15. DOI: 10.1111/bph.14664.

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## Kinase Inhibitor Library

Cat. No.: HY-L009

Product Name	Cat. No.	Compounds	Size (Pre-dissolved in DMSO/Solid)
Kinase Inhibitor Library	HY-L009	1,200+	30 µL/well, 50 µL/well, 100 µL/well, 250 µL/well (10 mM solution)

- A unique collection of 1,200+ phosphorylation kinase inhibitors/regulators for **high throughput screening (HTS)** and **high content screening (HCS)**.
- The library contains compounds targeting **protein kinases (VEGFR, EGFR, BTK, CDK, Akt, etc.)**, **lipid kinases (PI3K, PI4K, SK, etc.)** and **carbohydrate kinases (Hexokinase)**.
- Kinase inhibitors have played an increasingly prominent role in the treatment of cancer and other diseases.
- Bioactivity and safety confirmed by preclinical research and clinical trials. Some inhibitors have been approved by FDA.
- Structurally diverse, medicinally active, and cell permeable.
- Rich documentation with structure, IC<sub>50</sub>, and customer reviews.
- NMR and HPLC validated to ensure high purity.
- All compounds are in stock and continuously updated.

## Targets Included in Kinase Inhibitor Library:

ACK1	Adenosine Kinase	Akt	ALK	AMPK	Aurora Kinase	ATM/ATR
Axl	Bcr-Abl	BMX Kinase	Btk	CaMK-II	Casein Kinase	CDK
c-Fms	Checkpoint Kinase (Chk)	c-Kit	c-Met/HGFR	DAPK	DDR1/DDR2 Receptor	DNA-PK
DYRK	Ephrin Receptor	EGFR	ERK	FAK	FGFR	FLT3
GSK-3	Glucokinase	Haspin Kinase	IGF-1R	IKK	Insulin Receptor	IRAK
ITK	JAK	JNK	LIM Kinase(LIMK)	MAPKAPK2 (MK2)	MEK	MELK
MNK	Mixed Lineage Kinase	p38 MAPK	PAK	PDGFR	PDHK	PDK-1
PERK	PI3K	PI4K	PIKfyve	Pim	PKA	PKC
PKD	Polo-like Kinase (PLK)	Pyk2	Raf	Ribosomal S6 Kinase	RIP Kinase	ROCK
Ros1	Salt-inducible Kinases (SIKs)	SGK	SPHK	Src	SRPK	Syk
TAK1	Trk Receptor	ULK	VEGFR	Wee1	...	

 Publications Citing Use of MCE Kinase Library Inhibitors:

Nature. 2018 Aug;560(7719):499-503.

Nature. 2018 Jun;558(7711):540-546.

Science. 2017 Dec 1;358(6367).

Nat Med. 2019 Feb;25(2):292-300.

Nat Med. 2018 Aug;24(8):1143-1150.

Cell. 2018 Nov 1;175(4):984-997.e24.

Cell. 2018 Oct 4;175(2):442-457.e23.

Cell. 2018 Sep 20;175(1):171-185.e25.

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## You can select:

- ✓ Specific Compounds
- ✓ Quantities
- ✓ Plate Map
- ✓ Concentration
- ✓ Format (Dry/Solid or DMSO Solution)

## Apoptosis Compound Library

Cat. No.: HY-L003

Product Name	Cat. No.	Compounds	Size (Pre-dissolved in DMSO/Solid)
Apoptosis Compound Library	HY-L003	800+	30 µL/well, 50 µL/well, 100 µL/well, 250 µL/well (10 mM solution)

- A unique collection of **800+** small molecules used for survival, proliferation and apoptosis research.
- Targets such as **Bcl-2 Family, Caspase, DAPK, IAP, MDM2/p53, PKD, Survivin**, etc.
- Bioactivity and safety confirmed by preclinical research and clinical trials, some compounds have been approved by FDA.
- A useful tool to study apoptosis-involved regulation and diseases such as **cancer, aging, neurodegenerative disease**, and more.
- Structurally diverse, medicinally active, and cell permeable.
- More detailed compound information with structure, IC<sub>50</sub>, and other chemical & biological data.
- NMR and HPLC validated to ensure high purity and quality.
- All compounds are in stock and continuously updated.

### Targets Included in Apoptosis Compound Library:

Apoptosis	Bcl-2 Family	c-Myc	Caspase	DAPK
IAP	MDM-2/p53	PKD	RIP kinase	Survivin
Thymidylate Synthase	TNF-alpha			

### 📖 Publications Citing Use of MCE Apoptosis Library Compounds:

**Cell.** 2018 Sep 20;175(1):171-185.e25.

**Cancer Cell.** 2018 Aug 13;34(2):271-285.e7.

**Cell Metab.** 2019 Feb 14. pii: S1550-4131(19)30021-X.

**Cell Metab.** 2018 Oct. DOI: 10.2139/ssrn.3255557.

**Sci Transl Med.** 2018 Jul 18;10(450). pii: eaaq1093.

**Blood.** 2019 Jan 3;133(1):70-80.

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### Customize Library

#### You can select:

- ✓ Specific Compounds
- ✓ Quantities
- ✓ Plate Map
- ✓ Concentration
- ✓ Format (Dry/Solid or DMSO Solution)

## Autophagy Compound Library

Cat. No.: HY-L029

Product Name	Cat. No.	Compounds	Size (Pre-dissolved in DMSO/Solid)
Autophagy Compound Library	HY-L029	700+	30 $\mu$ L/well, 50 $\mu$ L/well, 100 $\mu$ L/well, 250 $\mu$ L/well (10 mM solution)

- A unique collection of 700+ small molecule compounds with biological activity used for **autophagy research and associated assays**.
- Targets include **Autophagy, LRRK2, and ULK**.
- A useful tool for the research of autophagy-related regulation and diseases.
- Bioactivity and safety confirmed by preclinical research and clinical trials. Some have been approved by FDA.
- Structurally diverse, medicinally active, and cell permeable.
- Detailed compound information with structure,  $IC_{50}$ , and brief introduction.
- Validated NMR and HPLC to ensure high purity and quality.
- All compounds are in stock and continuously updated.

### Targets Included in Autophagy Compound Library:

Autophagy                      LRRK2                      ULK

### Publications Citing Use of MCE Autophagy Library Compounds:

**Nature.** 2018 Nov;563(7729):131-136.

**Nature.** 2018 Aug;560(7719):499-503.

**Nat Med.** 2018 Aug;24(8):1143-1150.

**Cell.** 2019 Mar 7;176(6):1447-1460.e14.

**Cell.** 2019 Jan 24;176(3):505-519.e22.

**Cell.** 2018 Oct 4;175(2):442-457.e23.

**Cell.** 2018 Sep 20;175(1):186-199.e19.

**Cell.** 2018 Sep 20;175(1):171-185.e25.

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### Customize Library

#### You can select:

- ✓ Specific Compounds
- ✓ Quantities
- ✓ Plate Map
- ✓ Concentration
- ✓ Format (Dry/Solid or DMSO Solution)

## Cell Cycle/DNA Damage Compound Library

Cat. No.: HY-L004

Product Name	Cat. No.	Compounds	Size (Pre-dissolved in DMSO/Solid)
Cell Cycle/DNA Damage Compound Library	HY-L004	700+	30 µL/well, 50 µL/well, 100 µL/well, 250 µL/well (10 mM solution)

- A unique collection of 700+ Cell Cycle/DNA Damage related compounds for **high throughput screening (HTS)** and **high content screening (HCS)**.
- Targets such as **CDK, ROCK, Aurora Kinase, ATM/ATR, DNA-PK, DNA/RNA Synthesis**, etc.
- A useful tool to study the mechanism of cell cycle regulators that are critical to normal development and the development of **cancer, cardiovascular, inflammatory, and neurodegenerative diseases**.
- Bioactivity and safety confirmed by preclinical research and clinical trials. Some compounds have been approved by FDA.
- Structurally diverse, medicinally active, and cell permeable.
- More detailed compound information with structure, IC<sub>50</sub>, and other chemical & biological data.
- NMR and HPLC validated to ensure high purity and quality.
- All compounds are in stock and continuously updated.

### Targets Included in Cell Cycle/DNA Damage Compound Library:

Antifolate	APC	ATM/ATR	Aurora Kinase	Casein Kinase
CDK	Checkpoint Kinase (Chk)	CRISPR/Cas9	Deubiquitinase	DNA Alkylator/Crosslinker
DNA-PK	DNA/RNA Synthesis	G-quadruplex	Haspin Kinase	HDAC
HSP	Kinesin	KSP	LIM Kinase (LIMK)	Microtubule/Tubulin
Mps1	Nucleoside antimetabolite	p97	PAK	PARP
PERK	Polo-like Kinase (PLK)	PPAR	PTEN	RAD51
ROCK	Sirtuin	Telomerase	Topoisomerase	Wee1 ...

### Publications Citing Use of MCE Cell Cycle/DNA Damage Library Compounds:

**Nature.** 2018 Nov;563(7729):131-136.

**Nature.** 2017 Aug 24;548(7668):471-475.

**Science.** 2017 Dec 1;358(6367). pii: eaan4368.

**Nat Med.** 2019 Feb;25(2):292-300.

**Cell.** 2019 Mar 7;176(6):1447-1460.e14.

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### Customize Library

#### You can select:

- ✓ Specific Compounds
- ✓ Quantities
- ✓ Plate Map
- ✓ Concentration
- ✓ Format (Dry/Solid or DMSO Solution)

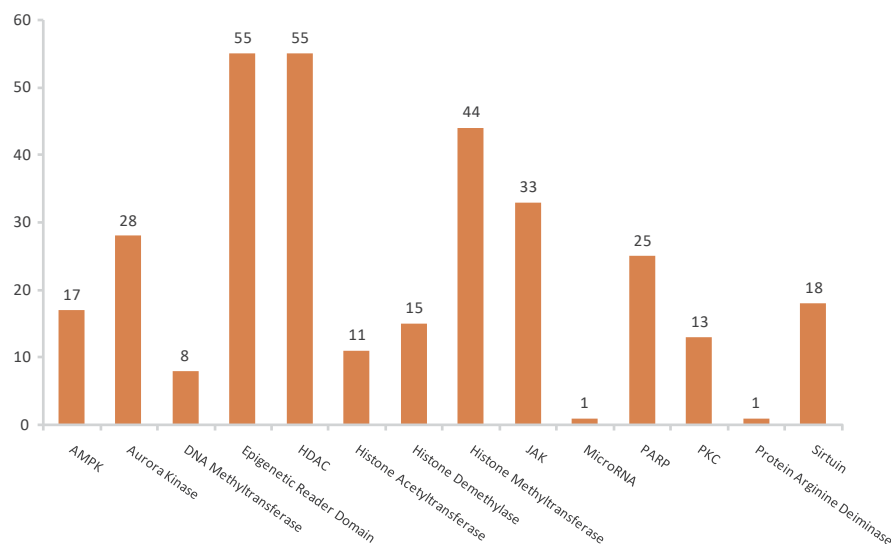
## Epigenetics Compound Library

Cat. No.: HY-L005

Product Name	Cat. No.	Compounds	Size (Pre-dissolved in DMSO/Solid)
Epigenetics Compound Library	HY-L005	400+	30 $\mu$ L/well, 50 $\mu$ L/well, 100 $\mu$ L/well, 250 $\mu$ L/well (10 mM solution)

- A unique collection of 400+ small molecule modulators with biological activity used for epigenetics research and associated assays.
- The library contains epigenetics-related compounds targeting HDAC, Histone Demethylase, Histone Acetyltransferase (HAT), DNA Methyltransferase (DNMT), Epigenetic Reader Domain, MicroRNA, etc.
- A valuable tool for chemical genomics, epigenetic target identification in pharmacogenomics, and other biological applications.
- Bioactivity and safety confirmed by preclinical research and clinical trials. Some compounds have been approved by FDA.
- Structurally diverse, medicinally active, and cell permeable.
- Rich documentation with structure,  $IC_{50}$ , and other chemical & biological data.
- NMR and HPLC validated to ensure the highest purity.
- All compounds are in stock and continuously updated.

Epigenetics Compound Library Composition



### Publications Citing Use of MCE Epigenetics Library Compounds:

Nat Med. 2018 Aug;24(8):1143-1150.  
 Cell. 2019 Jan 24;176(3):505-519.e22.  
 Cell. 2018 Sep 20;175(1):186-199.e19.  
 Cancer Discov. 2018 May;8(5):632-647.  
 Cancer Discov. 2018 May;8(5):616-631.  
 Cancer Discov. 2018 Mar;8(3):354-369.

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### Customize Library

#### You can select:

- ✓ Specific Compounds
- ✓ Quantities
- ✓ Plate Map
- ✓ Concentration
- ✓ Format (Dry/Solid or DMSO Solution)



## GPCR/G Protein Compound Library

Cat. No.: HY-L006

Product Name	Cat. No.	Compounds	Size (Pre-dissolved in DMSO/Solid)
GPCR/G Protein Compound Library	HY-L006	1,000+	30 µL/well, 50 µL/well, 100 µL/well, 250 µL/well (10 mM solution)

- A unique collection of **1,000+** small molecules targeting **G protein coupled receptors** used in GPCR screening for various research and drug development projects.
- Targets such as **5-HT Receptor, Dopamine Receptor, Opioid Receptor, Adrenergic Receptors, Cannabinoid Receptor, mGluR, ETA Receptor**, etc.
- The most successful class of drugable targets in the human genome and remain the most attractive family of targets.
- All of the small molecules in the GPCR library are well characterized with biological and pharmaceutical activity. Some compounds have been approved by the FDA.
- A powerful tool for discovering GPCR-based drugs that are the richest signal receptor targets for drug discovery.
- Structurally diverse, medicinally active, and cell permeable.
- Rich documentation with structure, IC<sub>50</sub>, and brief introduction.
- NMR and HPLC validated to ensure the highest purity.
- All compounds are in stock and continuously updated.

### Targets Included in GPCR/G Protein Compound Library:

5-HT Receptor	Adenosine Receptor	Adiponectin Receptor	Adrenergic Receptor	Angiotensin Receptor
Bombesin Receptor	Bradykinin Receptor	Cannabinoid Receptor	CaSR	CCR
CGRP Receptor	Cholecystokinin Receptor	CRTH2 (GPR44)	CXCR	Dopamine Receptor
EBI2/GPR183	Endothelin Receptor	GHSR	Glucagon Receptor	Glucocorticoid Receptor
GNRH Receptor	GPCR19	GPR109A	GPR119	GPR120
GPR139	GPR40	GPR55	GPR84	Histamine Receptor
Imidazoline Receptor	Leukotriene Receptor	LPL Receptor	mAChR	Melatonin Receptor
mGluR	Motilin Receptor	Neurokinin Receptor	Neuropeptide Y Receptor	Neurotensin Receptor
Opioid Receptor	Orexin Receptor (OX Receptor)	P2Y Receptor	Prostaglandin Receptor	Protease-Activated Receptors (PARs)
Ras	RGS	Sigma Receptor	TSH Receptor	Vasopressin Receptor ...

### Publications Citing Use of MCE GPCR/G Protein Library Compounds:

**Cell Metab.** 2018 Jul 3;28(1):118-129.e5.

**Immunity.** 2018 Nov 20;49(5):842-856.e7.

**Nat Cell Biol.** 2018 Oct;20(10):1145-1158.

**Cell Res.** 2019 Mar;29(3):193-205.

**Cell Res.** 2018 Mar;28(3):323-335.

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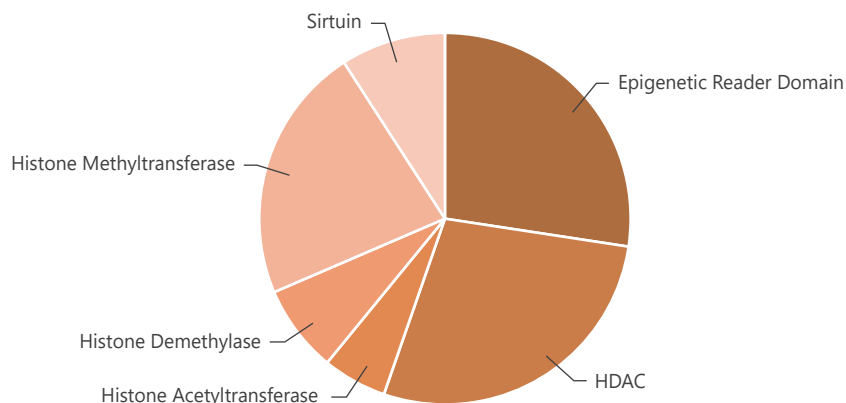
# Histone Modification Research Compound Library

Cat. No.: HY-L024

Product Name	Cat. No.	Compounds	Size (Pre-dissolved in DMSO/Solid)
Histone Modification Research Compound Library	HY-L024	300+	30 µL/well, 50 µL/well, 100 µL/well, 250 µL/well (10 mM solution)

- A unique collection of 300+ bioactive compounds for high throughput screening (HTS) and high content screening (HCS).
- Targets include Epigenetic Reader Domain, HDAC, Histone Acetyltransferase, Histone Demethylase, Histone Methyltransferase, Sirtuin, etc.
- A useful tool for the research of the regulation of histone modification and the corresponding diseases.
- Bioactivity and safety confirmed by preclinical research and clinical trials. Some inhibitors have been approved by FDA.
- Structurally diverse, medicinally active, and cell permeable.
- More detailed compound information with structure, IC<sub>50</sub>, and brief introduction.
- NMR and HPLC validated to ensure high purity and quality.
- All compounds are in stock and continuously updated.

Histone Modification Research Compound Library Composition



## Publications Citing Use of MCE Histone Modification Research Library Compounds:

Nat Med. 2017 Nov;23(11):1352-1361.

Cell. 2019 Mar 7;176(6):1447-1460.e14.

Cell. 2018 Sep 20;175(1):186-199.e19.

Cell Stem Cell. 2019 Mar 14. DOI: 10.1016/j.stem.2019.02.018.

Cancer Cell. 2018 Feb 12;33(2):274-291.e8.

Sci Transl Med. 2018 Jul 18;10(450).

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### Customize Library

#### You can select:

- ✓ Specific Compounds
- ✓ Quantities
- ✓ Plate Map
- ✓ Concentration
- ✓ Format (Dry/Solid or DMSO Solution)

## Immunology/Inflammation Compound Library

Cat. No.: HY-L007

Product Name	Cat. No.	Compounds	Size (Pre-dissolved in DMSO/Solid)
Immunology/Inflammation Compound Library	HY-L007	1,200+	30 µL/well, 50 µL/well, 100 µL/well, 250 µL/well (10 mM solution)

- A unique collection of **1,200+** small molecules with biological activity used for Immunology/Inflammation research.
- The library contains compounds targeting Immunology/Inflammation-related enzyme such as **CCR, COX, Interleukin Related, IRAK, MyD88, PDE, PD-1/PD-L1, TLR**, and more.
- A useful tool for researching the mechanism behind Immunology/Inflammation, drug screening and other pharmaceutical and biological applications.
- Bioactivity and safety confirmed by preclinical research and clinical trials. Some compounds have been approved by FDA.
- Structurally diverse, medicinally active, and cell permeable.
- Rich documentation with structure, IC<sub>50</sub>, and brief introduction.
- NMR and HPLC validated to ensure high purity and quality.
- All compounds are in stock and continuously updated.

### Targets Included in Immunology/Inflammation Compound Library:

CCR	COX	Complement System	CRTH2 (GPR44)	CXCR
FLAP	Histamine Receptor	IFNAR	Interleukin Related	IRAK
MyD88	NO Synthase	NOD-like Receptors (NLRs)	PD-1/PD-L1	PGE Synthase
Salt-inducible Kinases (SIKs)	SPHK	STING	Thrombopoietin Receptor	Toll-like Receptor (TLR)

### Publications Citing Use of MCE Immunology/Inflammation Library Compounds:

*Gastroenterology*. 2018 May;154(6):1822-1835.e2.

*Cell Res*. 2018 Mar;28(3):323-335.

*Circ Res*. 2018 May 25;122(11):1532-1544.

*Nat Microbiol*. 2017 May 15;2:17072.

*J Allergy Clin Immunol*. 2018 Jun;141(6):2286-2289.e5.

*Nat Commun*. 2019 Mar 4;10(1):1015.

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### Customize Library

#### You can select:

- ✓ Specific Compounds
- ✓ Quantities
- ✓ Plate Map
- ✓ Concentration
- ✓ Format (Dry/Solid or DMSO Solution)

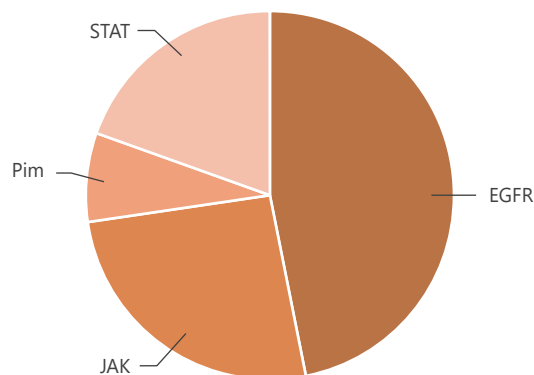
## JAK/STAT Compound Library

Cat. No.: HY-L008

Product Name	Cat. No.	Compounds	Size (Pre-dissolved in DMSO/Solid)
JAK/STAT Compound Library	HY-L008	200+	30 $\mu$ L/well, 50 $\mu$ L/well, 100 $\mu$ L/well, 250 $\mu$ L/well (10 mM solution)

- A unique collection of 200+ bioactive compounds related to JAK/STAT signaling used for high throughput screening (HTS) and high content screening (HCS).
- Targets include JAK, STAT, EGFR, Pim, etc.
- A useful tool for JAK/STAT-related drug discovery.
- Bioactivity and safety confirmed by preclinical research and clinical trials. Some inhibitors have been approved by FDA.
- Structurally diverse, medicinally active, and cell permeable.
- More detailed compound information with structure, IC<sub>50</sub>, and brief introduction.
- NMR and HPLC validated to ensure high purity and quality.
- All compounds are in stock and continuously updated.

JAK/STAT Compound Library Composition



### Publications Citing Use of MCE JAK/STAT Library Compounds:

Nat Med. 2018 Aug;24(8):1143-1150.

Cancer Discov. 2018 May;8(5):616-631.

Cancer Cell. 2018 Sep 10;34(3):439-452.e6.

Cancer Cell. 2018 Jun 11;33(6):1061-1077.

Nat Immunol. 2018 Mar;19(3):233-245.

Cell Metab. 2019 Jan 8;29(1):141-155.e9.

Sci Transl Med. 2018 Jul 18;10(450).

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### Customize Library

#### You can select:

- ✓ Specific Compounds
- ✓ Quantities
- ✓ Plate Map
- ✓ Concentration
- ✓ Format (Dry/Solid or DMSO Solution)

## MAPK Compound Library

Cat. No.: HY-L010

Product Name	Cat. No.	Compounds	Size (Pre-dissolved in DMSO/Solid)
MAPK Compound Library	HY-L010	200+	30 µL/well, 50 µL/well, 100 µL/well, 250 µL/well (10 mM solution)

- A unique collection of 200+ MAPK signaling inhibitors for **high throughput screening (HTS)** and **high content screening (HCS)**.
- Targets such as **ERK, JNK, MEK, p38 MAPK, Raf, RSK**, etc.
- A useful tool for MAPK-related drug discovery and disease research.
- Bioactivity and safety confirmed by preclinical research and clinical trials. Some inhibitors have been approved by FDA.
- Structurally diverse, medicinally active, and cell permeable.
- More detailed compound information with structure, IC<sub>50</sub>, and brief introduction.
- NMR and HPLC validated to ensure high purity and quality.
- All compounds are in stock and continuously updated.

### Targets Included in MAPK Compound Library:

ERK	JNK	KLF	MAPKAPK2 (MK2)	MEK
Mixed Lineage Kinase	MNK	p38 MAPK	Raf	Ribosomal S6 Kinase (RSK)

### Publications Citing Use of MCE MAPK Library Compounds:

**Science.** 2017 Dec 1;358(6367).

**Cell.** 2018 Aug 9;174(4):843-855.e19.

**Cancer Discov.** 2018 Sep;8(9):1130-1141.

**Cancer Discov.** 2018 Mar;8(3):354-369.

**Nat Immunol.** 2018 Mar;19(3):233-245.

**Cell Metab.** 2019 Jan 8;29(1):141-155.e9.

**Sci Transl Med.** 2019 Feb 6;11(478).

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### Customize Library

#### You can select:

- ✓ Specific Compounds
- ✓ Quantities
- ✓ Plate Map
- ✓ Concentration
- ✓ Format (Dry/Solid or DMSO Solution)

## Membrane Transporter/Ion Channel Compound Library

Cat. No.: HY-L011

Product Name	Cat. No.	Compounds	Size (Pre-dissolved in DMSO/Solid)
Membrane Transporter/Ion Channel Compound Library	HY-L011	500+	30 $\mu$ L/well, 50 $\mu$ L/well, 100 $\mu$ L/well, 250 $\mu$ L/well (10 mM solution)

- A unique collection of 500+ small molecule modulators used for Ion Channel and Membrane Transporter research.
- The library contains compounds targeting Membrane Transporters including Pgp, CRM1, BCRP, etc., and Ion Channels including CFTR, proton pump, sodium pump, calcium pump, etc.
- A useful tool for the research of drug absorption and distribution.
- Bioactivity and safety confirmed by preclinical research and clinical trials. Some inhibitors have been approved by FDA.
- Structurally diverse, medicinally active, and cell permeable.
- Rich documentation with structure, IC<sub>50</sub>, and summary.
- NMR and HPLC validated to ensure high purity.
- All compounds are in stock and continuously updated.

### Targets Included in Membrane Transporter/Ion Channel Compound Library:

ATP Synthase	BCRP	Calcium Channel	CFTR	Chloride Channel
CRAC Channel	CRM1	EAAT2	GABA Receptor	GlyT
HCN Channel	iGluR	Monoamine transporter	Monocarboxylate Transporter	Na <sup>+</sup> /Ca <sup>2+</sup> Exchanger
Na <sup>+</sup> /HCO <sub>3</sub> <sup>-</sup> Cotransporter	Na <sup>+</sup> /K <sup>+</sup> ATPase	nAChR	NKCC	P-glycoprotein
P2X Receptor	Potassium Channel	Proton Pump	SGLT	Sodium Channel
TRP Channel	URAT1	VDAC		

### Publications Citing Use of MCE Membrane Transporter/Ion Channel Library Compounds:

**Nature.** 2018 Aug;560(7719):499-503.

**Nat Med.** 2019 Feb;25(2):337-349.

**Clin Cancer Res.** 2018 Jan 15;24(2):383-394.

**PLoS Biol.** 2018 Jul 12;16(7):e2004921.

**Cell Syst.** 2018 Apr 25;6(4):424-443.e7.

**Theranostics.** 2018 Oct 29;8(19):5452-5468.

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### Customize Library

#### You can select:

- ✓ Specific Compounds
- ✓ Quantities
- ✓ Plate Map
- ✓ Concentration
- ✓ Format (Dry/Solid or DMSO Solution)

## Metabolism/Protease Compound Library

Cat. No.: HY-L012

Product Name	Cat. No.	Compounds	Size (Pre-dissolved in DMSO/Solid)
Metabolism/Protease Compound Library	HY-L012	1,400+	30 µL/well, 50 µL/well, 100 µL/well, 250 µL/well (10 mM solution)

- A unique collection of **1,400+** Metabolism/Protease-related small molecules for **high throughput screening (HTS)** and **high content screening (HCS)**.
- Targets such as **PDE, Cytochrome P450, HMG-CoA Reductase, DPP4, Proteasome, HCV Protease, IDO, Cathepsin, MMP**, etc.
- A useful tool for drug discovery of metabolism-related diseases.
- Bioactivity and safety confirmed by preclinical research and clinical trials. Some inhibitors have been approved by FDA.
- Structurally diverse, medicinally active, and cell permeable.
- More detailed compound information with structure, IC<sub>50</sub>, and brief introduction.
- NMR and HPLC validated to ensure high purity and quality.
- All compounds are in stock and continuously updated.

### Targets Included in Metabolism/Protease Compound Library:

15-PGDH	5 alpha Reductase	5-Lipoxygenase	Adenosine Deaminase
Aldehyde Dehydrogenase (ALDH)	Aldose Reductase	Aminopeptidase	Angiotensin-converting Enzyme (ACE)
Carbonic Anhydrase	Carboxypeptidase	Cathepsin	DGAT
Cytochrome P450	Dipeptidyl Peptidase	Elastase	E1/E2/E3 Enzyme
FAAH	Factor Xa	Farnesyl Transferase	Fatty Acid Synthase (FAS)
Glucokinase	HCV Protease	HIF/HIF Prolyl-Hydroxylase	HIV Integrase
HIV Protease	HMG-CoA Reductase (HMGCR)	HSP	Indoleamine 2,3-Dioxygenase (IDO)
Isocitrate Dehydrogenase (IDH)	MAGL	MMP	Nampt
PAI-1	Phosphodiesterase (PDE)	Procollagen C Proteinase	Proteasome
Pyruvate Dehydrogenase	Renin	Ser/Thr Protease	Stearoyl-CoA Desaturase (SCD)
Thrombin	Tryptophan Hydroxylase	Tyrosinase	Xanthine Oxidase ...

### Publications Citing Use of MCE Metabolism/Protease Library Compounds:

Science. 2018 Sep 28;361(6409).

Cell. 2018 Aug 9;174(4):843-855.e19.

Nat Methods. 2018 Jul;15(7):519-522.

Cancer Cell. 2018 Sep 10;34(3):411-426.e19.

Cell Host Microbe. 2018 Sep 12;24(3):353-363.e5.

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## Neuronal Signaling Compound Library

Cat. No.: HY-L013

Product Name	Cat. No.	Compounds	Size (Pre-dissolved in DMSO/Solid)
Neuronal Signaling Compound Library	HY-L013	1,000+	30 µL/well, 50 µL/well, 100 µL/well, 250 µL/well (10 mM solution)

- A unique collection of 1,000+ Neuronal Signaling-related compounds for high throughput screening (HTS) and high content screening (HCS).
- Targets such as 5-HT Receptor, AChE, Adrenergic Receptor, AMPAR, Beta-secretase, Dopamine Receptor, FAAH, Melatonin Receptor, AChR, Opioid Receptor,  $\gamma$ -secretase, etc.
- A useful tool for the research of neuronal regulation and neuronal diseases.
- Bioactivity and safety confirmed by preclinical research and clinical trials. Some inhibitors have been approved by FDA.
- Structurally diverse, medicinally active, and cell permeable.
- More detailed compound information with structure,  $IC_{50}$ , and brief introduction.
- NMR and HPLC validated to ensure high purity and quality.
- All compounds are in stock and continuously updated.

### Targets Included in Neuronal Signaling Compound Library:

5-HT Receptor	AChE	Adenosine Kinase	Amyloid- $\beta$	Beta-secretase
CaMK	CGRP Receptor	COMT	Dopamine Receptor	Dopamine Transporter
FAAH	GABA Receptor	GlyT	iGluR	Imidazoline Receptor
mAChR	Melatonin Receptor	Monoamine Oxidase	nAChR	Neurokinin Receptor
Opioid Receptor	Serotonin Transporter	$\gamma$ -secretase		

### Publications Citing Use of MCE Neuronal Signaling Library Compounds:

Nat Med. 2019 Feb;25(2):337-349.

Sci Transl Med. 2019 Feb 6;11(478).

Cell Res. 2018 Dec;28(12):1171-1185.

J Clin Invest. 2018 Jan 2;128(1):483-499.

Nat Commun. 2018 Apr 26;9(1):1677.

Cell Syst. 2018 Apr 25;6(4):424-443.e7.

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### Customize Library

#### You can select:

- ✓ Specific Compounds
- ✓ Quantities
- ✓ Plate Map
- ✓ Concentration
- ✓ Format (Dry/Solid or DMSO Solution)



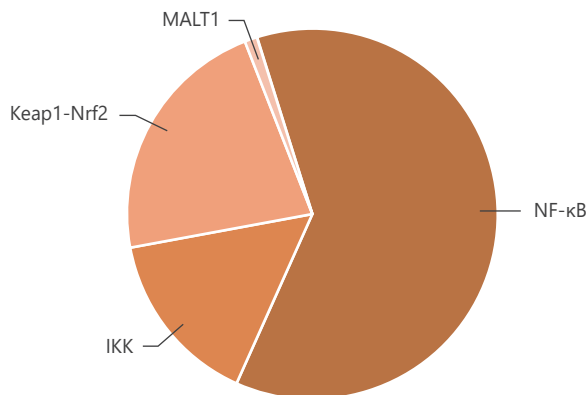
## NF-κB Signaling Compound Library

Cat. No.: HY-L014

Product Name	Cat. No.	Compounds	Size (Pre-dissolved in DMSO/Solid)
NF-κB Signaling Compound Library	HY-L014	200+	30 μL/well, 50 μL/well, 100 μL/well, 250 μL/well (10 mM solution)

- A unique collection of 200+ NF-κB signaling related small molecule compounds for **high throughput screening (HTS)** and **high content screening (HCS)**.
- Targets such as **IKK, Keap1-Nrf2, NF-κB**, etc.
- A powerful tool for researching the mechanism behind cancer, drug screening based on NF-κB signaling pathway and other pharmaceutical and biological applications.
- Bioactivity and safety confirmed by preclinical research and clinical trials. Some inhibitors have been approved by FDA.
- Structurally diverse, medicinally active, and cell permeable.
- More detailed compound information with structure, IC<sub>50</sub>, and brief introduction.
- NMR and HPLC validated to ensure high purity and quality.
- All compounds are in stock and continuously updated.

NF-κB Signaling Compound Library Composition



### Publications Citing Use of MCE NF-κB Signaling Library Compounds:

**Nat Med.** 2018 Aug;24(8):1143-1150.

**Gut.** 2018 Nov;67(11):2035-2044.

**Sci Transl Med.** 2018 Jul 18;10(450).

**Cell Res.** 2019 Mar;29(3):193-205.

**Cell Res.** 2018 Dec;28(12):1171-1185.

**Nat Commun.** 2018 Oct 24;9(1):4429.

**Proc Natl Acad Sci U S A.** 2019 Feb 19;116(8):2996-3005.

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## PI3K/Akt/mTOR Compound Library

Cat. No.: HY-L015

Product Name	Cat. No.	Compounds	Size (Pre-dissolved in DMSO/Solid)
PI3K/Akt/mTOR Compound Library	HY-L015	200+	30 $\mu$ L/well, 50 $\mu$ L/well, 100 $\mu$ L/well, 250 $\mu$ L/well (10 mM solution)

- A unique collection of 200+ small molecule inhibitors used for PI3K/Akt/mTOR pathway research.
- Targets such as Akt, AMPK, DNA-PK, PDK-1, mTOR, PI3K, PTEN, etc.
- A valuable tool for studying PI3K/Akt/mTOR-related survival, proliferation, and apoptosis of cells and related diseases.
- Bioactivity and safety confirmed by preclinical research and clinical trials. Some inhibitors have been approved by the FDA.
- Structurally diverse, medicinally active, and cell permeable.
- Rich documentation with structure, IC<sub>50</sub>, and summary.
- NMR and HPLC validated to ensure high purity.
- All compounds are in stock and continuously updated.

### Targets Included in PI3K/Akt/mTOR Compound Library:

Akt	AMPK	ATM/ATR	DNA-PK	GSK-3	MELK
mTOR	PDK-1	PI3K	PI4K	PIKfyve	PTEN

### Publications Citing Use of MCE PI3K/Akt/mTOR Library Compounds:

**Nature.** 2018 Aug;560(7719):499-503.

**Nature.** 2018 Jun;558(7711):540-546.

**Cancer Discov.** 2018 May;8(5):632-647.

**Cancer Discov.** 2018 Mar;8(3):354-369.

**Cell Stem Cell.** 2018 Mar 1;22(3):369-383.e8.

**Cancer Cell.** 2018 Jun 11;33(6):1061-1077.e6.

**J Med Chem.** 2018 Jan 11;61(1):360-371.

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### Customize Library

#### You can select:

- ✓ Specific Compounds
- ✓ Quantities
- ✓ Plate Map
- ✓ Concentration
- ✓ Format (Dry/Solid or DMSO Solution)

## Protein Tyrosine Kinase Compound Library

Cat. No.: HY-L016

Product Name	Cat. No.	Compounds	Size (Pre-dissolved in DMSO/Solid)
Protein Tyrosine Kinase Compound Library	HY-L016	400+	30 µL/well, 50 µL/well, 100 µL/well, 250 µL/well (10 mM solution)

- A unique collection of 400+ protein kinase inhibitors for **high throughput screening (HTS)** and **high content screening (HCS)**.
- Targets such as **VEGFR, ALK, Btk, Bcr-Abl, c-Met/HGFR, EGFR, FGFR, Insulin Receptor, JAK, PDGFR**, etc.
- A useful tool for the research for PTK-related diseases, such as cancer.
- Bioactivity and safety confirmed by preclinical research and clinical trials. Some protein kinase inhibitors have been approved by FDA.
- Structurally diverse, medicinally active and cell permeable.
- Rich documentation with structure, IC<sub>50</sub> and summary.
- NMR and HPLC to ensure the high purity.
- All compounds are in stock and continuously updated.

### Targets Included in Protein Tyrosine Kinase Compound Library:

Ack1	ALK	Bcr-Abl	BMX Kinase	Btk	c-Fms
c-Kit	c-Met/HGFR	Discoidin Domain Receptor	DYRK	EGFR	Ephrin Receptor
FAK	FGFR	FLT3	IGF-1R	Insulin Receptor	IRAK
Itk	PDGFR	PKA	Pyk2	ROS	Src
Syk	TAM Receptor	Trk Receptor	VEGFR		

### Publications Citing Use of MCE Protein Tyrosine Kinase Library Compounds:

**Nature.** 2017 Aug 24;548(7668):471-475.

**Science.** 2017 Dec 1;358(6367).

**Nat Med.** 2017 Nov;23(11):1319-1330.

**Cell.** 2018 Oct 4;175(2):442-457.e23.

**Cancer Discov.** 2018 Jun;8(6):714-729.

**Cancer Discov.** 2018 Mar;8(3):354-369.

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### Customize Library

#### You can select:

- ✓ Specific Compounds
- ✓ Quantities
- ✓ Plate Map
- ✓ Concentration
- ✓ Format (Dry/Solid or DMSO Solution)

## Stem Cell Signaling Compound Library

Cat. No.: HY-L017

Product Name	Cat. No.	Compounds	Size (Pre-dissolved in DMSO/Solid)
Stem Cell Signaling Compound Library	HY-L017	300+	30 $\mu$ L/well, 50 $\mu$ L/well, 100 $\mu$ L/well, 250 $\mu$ L/well (10 mM solution)

- A unique collection of 300+ small molecule inhibitors with biological activity used for stem cell regulatory and signaling pathway research.
- Targets such as GSK-3, Hedgehog, Notch, JAK, ROCK, Wnt,  $\gamma$ -secretase, Casein Kinase, etc.
- A powerful tool for researching the mechanism behind stem cells, regenerative therapy, drug screening based on tumor stem cells, as well as other pharmaceutical and biological applications.
- Bioactivity and safety confirmed by preclinical research and clinical trials. Some protein kinase inhibitors have been approved by FDA.
- Structurally diverse, medicinally active, and cell permeable.
- Rich documentation with structure, IC<sub>50</sub>, and customer reviews.
- NMR and HPLC validated to ensure the highest purity.
- All compounds are in stock and continuously updated.

### Targets Included in Stem Cell Signaling Compound Library:

Casein Kinase	ERK	Gli	GSK-3	Hedgehog	Hippo (MST)
JAK	Notch	Oct3/4	PKA	Porcupine	ROCK
sFRP-1	Smo	STAT	TGF-beta/Smad	Wnt	YAP
$\beta$ -catenin	$\gamma$ -secretase				

### Publications Citing Use of MCE Stem Cell Signaling Library Compounds:

**Nature.** 2017 May 18;545(7654):355-359.  
**Nat Med.** 2018 Nov;24(11):1752-1761.  
**Nat Med.** 2018 Aug;24(8):1143-1150.  
**Cell.** 2018 Jul 26;174(3):636-648.e18.  
**Cancer Discov.** 2018 May;8(5):616-631.  
**Cancer Cell.** 2018 Sep 10;34(3):439-452.e6.  
**Cell Metab.** 2019 Jan 8;29(1):141-155.e9.  
**Sci Transl Med.** 2018 Jul 18;10(450).

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### Customize Library

#### You can select:

- ✓ Specific Compounds
- ✓ Quantities
- ✓ Plate Map
- ✓ Concentration
- ✓ Format (Dry/Solid or DMSO Solution)

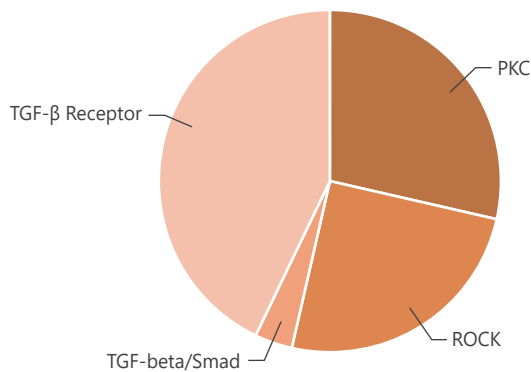
## TGF-beta/Smad Compound Library

Cat. No.: HY-L018

Product Name	Cat. No.	Compounds	Size (Pre-dissolved in DMSO/Solid)
TGF-beta/Smad Compound Library	HY-L018	100+	30 µL/well, 50 µL/well, 100 µL/well, 250 µL/well (10 mM solution)

- A unique collection of 100+ TGF-beta/Smad inhibitors for high throughput screening (HTS) and high content screening (HCS).
- Targets include PKC, ROCK, TGF-beta/Smad, and TGF-β Receptor.
- A useful tool for researching TGF-beta/Smad-related regulation and diseases.
- Bioactivity and safety confirmed by preclinical research and clinical trials. Some inhibitors have been approved by FDA.
- Structurally diverse, medicinally active, and cell permeable.
- More detailed compound information with structure, IC<sub>50</sub>, and brief introduction.
- NMR and HPLC validated to ensure high purity and quality.
- All compounds are in stock and continuously updated.

TGF-beta/Smad Compound Library Composition



 Publications Citing Use of MCE TGF-beta/Smad Library Compounds:

Bone Res. 2019 Mar 6;7:8.

Cell Syst. 2018 Apr 25;6(4):424-443.e7.

Biomaterials. 2018 Dec 6;193:30-46.

Cell Rep. 2019 Feb 12;26(7):1709-1717.e3.

Cell Rep. 2019 Jan 8;26(2):407-414.e5.

J Autoimmun. 2018 May;89:125-138.

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## Wnt/Hedgehog/Notch Compound Library

Cat. No.: HY-L020

Product Name	Cat. No.	Compounds	Size (Pre-dissolved in DMSO/Solid)
Wnt/Hedgehog/Notch Compound Library	HY-L020	100+	30 µL/well, 50 µL/well, 100 µL/well, 250 µL/well (10 mM solution)

- A unique collection of 100+ small molecule inhibitors with biological activity used for Wnt/Hedgehog/Notch pathway research and screening.
- Targets include **Notch, Gli, GSK-3, Hedgehog, Porcupine, sFRP-1, Smo, Wnt, β-catenin**, etc.
- A useful tool for the research of Wnt/Hedgehog/Notch-related regulation and diseases.
- Bioactivity and safety confirmed by preclinical research and clinical trials. Some inhibitors have been approved by FDA.
- Structurally diverse, medicinally active, and cell permeable.
- More detailed compound information with structure, IC<sub>50</sub>, and brief introduction.
- NMR and HPLC validated to ensure high purity and quality.
- All compounds are in stock and continuously updated.

### Targets Included in Wnt/Hedgehog/Notch Compound Library:

Casein Kinase	Gli	GSK-3	Hedgehog	Notch	Porcupine
sFRP-1	Smo	TGF-beta/Smad	Wnt	YAP	β-catenin

### Publications Citing Use of MCE Wnt/Hedgehog/Notch Library Compounds:

Nature. 2017 May 18;545(7654):355-359.

Nat Med. 2018 Nov;24(11):1752-1761.

Mol Cell. 2019 Jan 3;73(1):7-21.e7.

EMBO Mol Med. 2018 Nov;10(11).

Proc Natl Acad Sci U S A. 2018 Aug 7;115(32):E7522-E7531.

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### Customize Library

#### You can select:

- ✓ Specific Compounds
- ✓ Quantities
- ✓ Plate Map
- ✓ Concentration
- ✓ Format (Dry/Solid or DMSO Solution)

## Virtual Screening

Virtual screening is a computational technique used to search libraries of small molecules in order to identify those structures which are most likely to bind to a drug target. Nowadays, it has become a crucial step in early-stage drug discovery owing to its unique advantages over experimental HTS: drug target-relevant, competitive price and efficient.

MedChemExpress (MCE) provides high quality virtual screening service that enables researchers to identify most promising candidates.

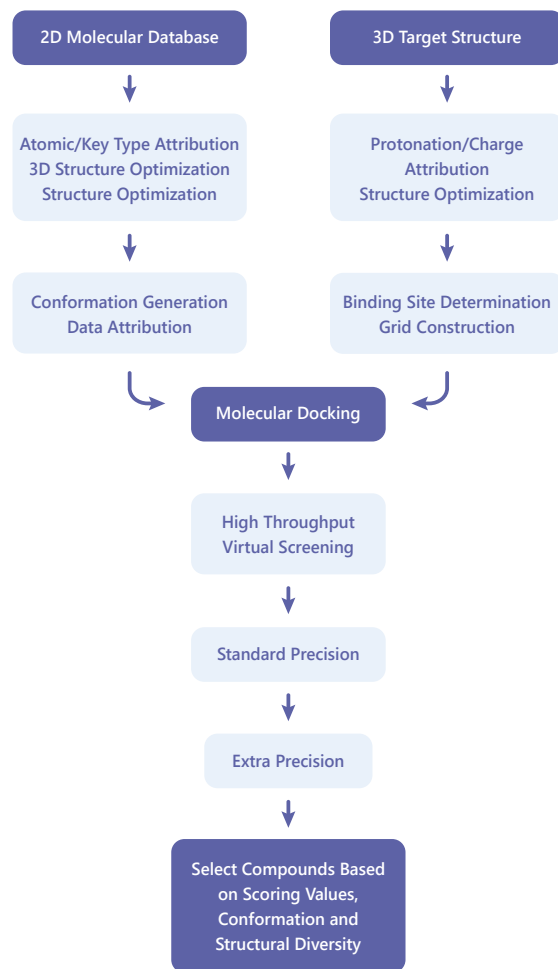
The virtual screening methods are mainly divided into two types: structure-based virtual screening (SBVS) and ligand-based virtual screening (LBVS).

### • SBVS

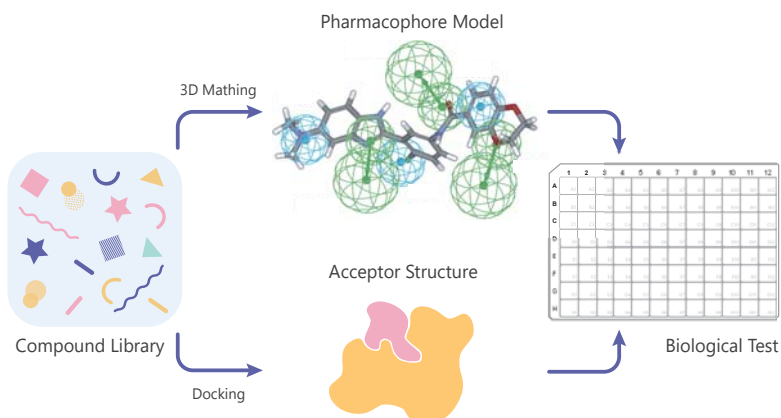
The general scheme of a SBVS strategy starts with processing the 3D target structural information of pharmaceutical protein interested (determined either experimentally or computationally through homology modeling) and then dock the small molecules to targeted binding sites. These docked compounds are then ranked based on their predicted binding affinity or complementarity to the binding site, as well as other criteria. Usually only a few top-ranked compounds are selected as candidates for further experimental assays. Our fast and accurate ligand docking and scoring procedures lead to efficient virtual screening.

### • LBVS

In the absence of 3D structures of potential drug targets, LBVS is one of the most popular approaches for drug discovery and lead optimization. Biological data are explored in order to identify known active or inactive compounds that will be used to retrieve other potentially active molecular scaffolds for experimental evaluation. LBVS methods include approaches such as similarity and substructure searching, quantitative structure-activity relationships (QSAR), pharmacophore mapping, and machine learning.



MCE SBVS Protocol



### Advantages:

- Ligand-based and structure-based virtual screening
- Super high-performance computer
- Compound database containing over 2 million purchasable compounds
- 3D pharmacophore model building
- Consideration of water and solvation effects

Product Name	Compounds	Features
MCE Bioactive Compound Library	9,000+	A unique collection of 9,000+ bioactive and structurally diverse compounds. Bioactivity and safety confirmed by preclinical research and clinical trials. Some have been approved by FDA.
MCE Fragment Library	8,000+	Latest release of Ro3 Fragment Library comprising over 8,000+ high-quality molecules. A useful tool for the fragment-based approach to drug discovery (FBDD).
HTS Compound Library	2,157,315	Enamine HTS Collection contains 2,157,315 diverse screening compounds. These compounds frequently have unusual structures and unique properties. The collection is particularly recommended for the researchers looking for most diverse screening set.
Advanced Library	459,417	Enamine Advanced Collection contains 459,417 compounds that have lead-like properties with MW $\leq$ 350, ClogP $\leq$ 3, and RotBonds $\leq$ 7 and/or valuable pharmacophores such as carboxylic, primary amino and amide groups.
Premium Library	43,408	Enamine Premium Collection contains over 43,408 compounds having most favorable molecular properties (high Fsp3, low logP and MW).
Agro-like Library	15,085	Library of compounds intended for use in agro/crop science.
Allosteric GPCR Library	14,535	A sub-library of Enamine's GPCR Library designed for discovery of novel allosteric ligands.
Allosteric Kinase Library	4,800	Carefully selected molecules via docking and visual evaluation.
Antiviral Library	3,700	Nucleoside-like compounds able to act as antiviral.
Aquaporins Library	1,500	A unique collection of 1,500 bioactive compounds targeting aquaporins.
BACE Library	7,171	The library was designed to find molecules which target Beta-secretase (BACE).
CNS Library	38,080	Library of novel small molecules with high CNS MPO scores.
Covalent Screening Library	14,249	A set of screening compounds bearing "warheads" for covalent target modification.
Discovery Diversity Set 10	10,560	Enamine Discovery Diversity Sets (DDS) are high-quality compound libraries focused on novel chemotypes and non-trivial structures. They compose of DDS-10 (10,560 compounds) and DDS-50 (50,240 compounds) sets which do not overlap. Discovery Diversity Set 10 contains 10,560 diverse screening compounds.
Discovery Diversity Set 50	50,240	Enamine Discovery Diversity Sets (DDS) are high-quality compound libraries focused on novel chemotypes and non-trivial structures. They compose of DDS-10 (10,560 compounds) and DDS-50 (50,240 compounds) sets which do not overlap. Discovery Diversity Set 50 contains 50,240 diverse screening compounds.
DNA Library	5,530	Designed for identification of new actives against proteins essential for DNA stability.
Epigenetics Library	9,353	Library of compounds focusing to hit on a number of epigenetic targets.
Glycomimetic Library	2,718	Specially synthesized set of compounds able to mimic glycosides and their interaction with proteins.
GPCR Library	54,080	Designed for discovery of new GPCR ligands.
Hit Locator Library 300	300,115	Enamine Hit Locator Library (HLL) is a sizable highly diverse screening set of 500,160 novel screening compounds. Hit Locator Library 300 (Core Set) contains 300,115 core compounds.
Hit Locator Library 500	500,160	Enamine Hit Locator Library (HLL) is a sizable highly diverse screening set of 500,160 novel screening compounds. Hit Locator Library 500 (Entire Set) contains 500,160 compounds.
IDO Targeted Library	5,502	IDO focused library designed by a combination of structure- and ligand-based methods.
Immuno-Oncology Library	52,935	Designed for discovery of novel hits in Immuno-Oncology therapeutic area.
Ion Channel Library	36,800	Designed for discovery of new Ion Channels ligands.
Protein-Protein Interaction Library	40,640	Designed for discovery of novel PPI inhibitors.
Specs HTS Compounds Library	210,070	Specs HTS library is a unique collection contains 210,070 diverse screening compounds for the lead identification via high-throughput screening (HTS) and high content screening (HCS).



## About Us

### Overview of MedChemExpress

MedChemExpress (MCE) offers a wide range of high quality research chemicals and biochemicals including novel life-science reagents, reference compounds, APIs and natural compounds for laboratory and scientific use. MCE has knowledgeable and friendly customer service and technical support teams with years of experience in the life science industry. MCE will be a competent and trustworthy partner for your research and scientific projects.

### Quality

Product quality is the key to our success and we take pride in offering only the highest-grade products. Product identity, quality, purity and activity are assured by our robust quality control and assurance policies, programs and procedures. We perform thorough analytical testing - including HNMR, LC-MS and HPLC - stability testing and activity assays on our products and the results from these tests are available to clients.

### Experience

Our chemists are highly experienced in molecular synthesis and the preparation of large quantities of structurally diverse and synthetically challenging molecules. We work with clients that have widely different needs and we have been very successful in meeting such needs.

### Services

We offer:

- Structurally and synthetically diverse biologically active compounds
- Flexible order volume ranging from milligrams to kilograms scale
- On-time delivery of products

We are a client-centric company and are always looking to hearing from you about how our products and services might better assist you.

For More Product Information, Please Visit Us Online

[www.MedChemExpress.com](http://www.MedChemExpress.com)



www.MedChemExpress.com

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