TargetMol®

A DRUG SCREENING EXPERT

COMPOUND LIBRARY

Bioactive Compound Library
Natural Product Library
Approved Drug Library
Fragment Library

◉ Ⅰ Bioactive Compound Libraries

For drug screening, cell induction, drug repurposing, mechanism research, target identification, positive control and other related research fields.

1.1 Library Categories based on Marketing Status

1.2 COVID-19-related Compound Libraries

1.3 Disease-related Compound Libraries

1.4 Library Categories based on Targets in Signaling Pathway

1.5 Characteristic Bioactive Libraries

◉ Ⅱ Natural Product Libraries

For cell induction research and drug screening focused on unique natural structures with new bioactivity.

2.1 Natural Product Library for HTS

2.2 Characteristic Natural Product Libraries

2.3 Natural Product Derivatives Library

2.4 Selectable Natural Product Library

◉ Ⅲ Fragment Libraries

For various fragment-based drug design and new drug discovery.

3.1 Featured Fragment Libraries

◉ IV Scaffold and Scaffold-based Libraries

A powerful tool for drug design and new drug discovery.

◉ V Custom Library

Select compounds, quantities, plate map, concentration and format (dry/solid or DMSO) to meet your specific requirement.
Please contact us at info@targetmol.com to customize your library.

Select

The quantity and price of compounds are subject to our dynamically updating official website.

TargetMol®
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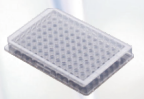
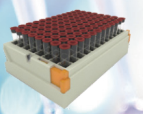
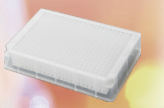
Documentation for TargetMol® Compound Library

Plate layout data is provided along with all library shipments and includes：

Excel： .xls(spreadsheet)file that includes all non-structural fields of the SD files.
SD file: Containing each chemical structure with the following information: unique TargetMol® ID number, plate or box ID value, column location, row location, coordinates(column and row locations combined), MW value, amount of compound and additional descriptions. Discovery Studio is the recommended software to open the SD files.
QA and instruction： Containing the compound libraries instructions.

Package format	96-well plate	96-Well deep-well plate	384-well plate
Quantity	⩽ 50pl	>50μL	By customer request
Plate type	V Shape，PP，0.36ml	V Bottom，PP，2D barcoded，SepraSeal Cap, 1.4mL	V Shape，PP，0.24ml
Size/ solvent	10 mM DMSO	10 mM DMSO	10 mM DMSO
Storage	-20°C (shipping or short-term preservation) -80°C (long-term preservation)		
			

Library Categories based on Marketing Status

Approved Drug Library

Catalog No. L1000 — 2356 compounds

Product Description

Traditional de novo drug discovery and development involves an HTS campaign for de novo candidate hits and requires highly specialized screening facilities and compound libraries containing several million compounds. It is a time-consuming and expensive process. As the regulation for drug safety and efficacy is increasingly complex, the cost of developing new drugs is skyrocketing. Drug repurposing, also known as the new use of old drugs, is an effective strategy to find new indications for existing drugs. It has recently drawn attention and led to several blockbuster drugs because of its high efficiency and low-cost. High-content screenings, new biomarkers, noninvasive imaging techniques, and advances in bioinformatics have created new opportunities for pursuing novel indications for approved compounds.
Approved drugs have known and well-characterized bioactivities, safety and bioavailability – properties that could dramatically accelerate drug development and optimization. Hits from this set will provide a significant head start in any drug optimization program.
In addition, a growing number of compounds have been identified from this library that can functionally replace reprogramming transcription factors, enhance the efficiency of iPSC generation and accelerate the reprogramming process by single use or a combination of several molecules.
For peptides and other drug molecules with low solution stability, we provide them in the form of dry powder (set as Part B) to ensure the optimum condition of our compound library and increase the probability of successful screening.

Product Advantage

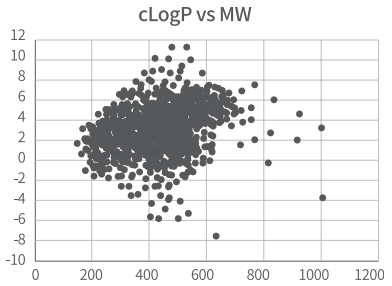
- A unique collection of 2356 approved drugs; a powerful tool for drug repurposing and cell differentiation induction;
- Covers various research areas, such as Cancer, Cardiovascular disease, Neuroscience, Immunology/Inflammation, etc.
- Detailed compound information with structure, target, activity, IC50 value, and brief introduction;
- NMR and HPLC/LCMS were validated to ensure high purity and quality and reduce false positive rates.

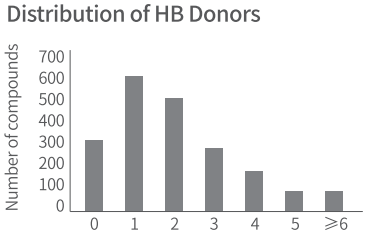
Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	11,780.00
250 µL * 10 mM (in DMSO)	USD	23,424.00
1 mg	USD	23,424.00

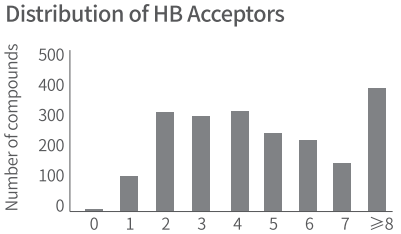
Drug-Like Properties

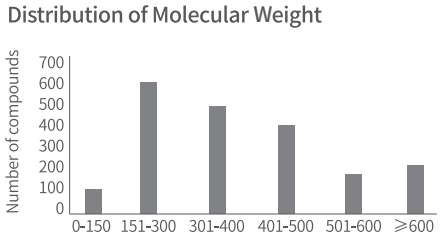
% of compounds compliant with Lipinski's Rules

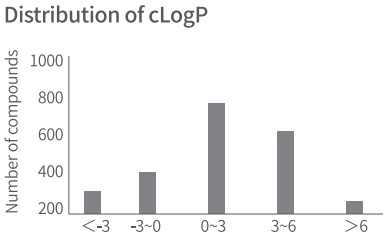
PhysChem Properties	% Compounds
<5 H-Bond donors	88
<10 H-Bond acceptors	90
cLogP<5	90
MW<500	79



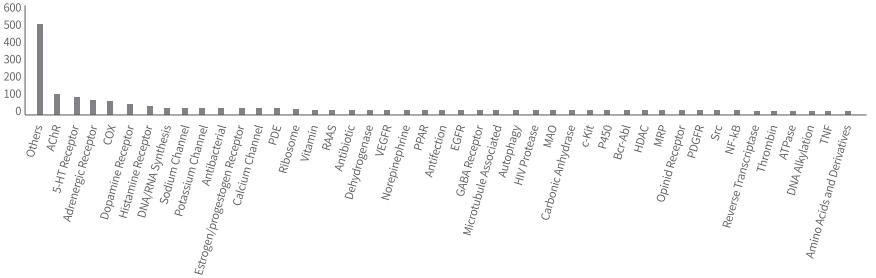




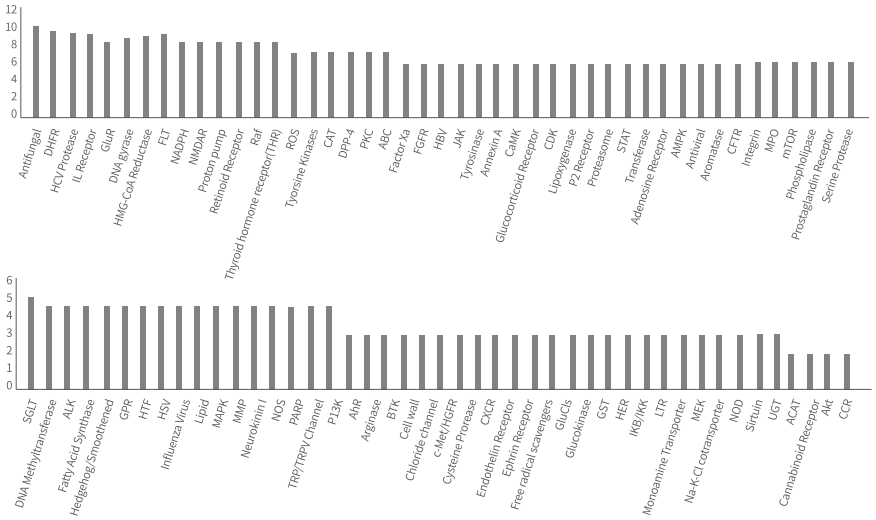




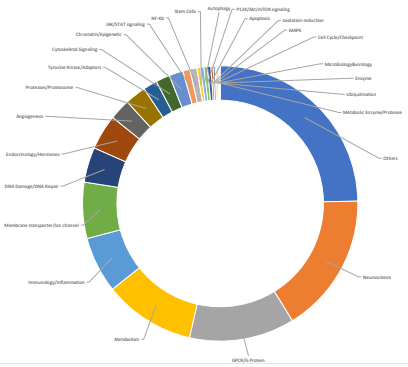
Target Composition



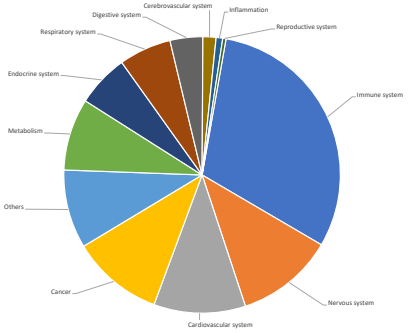
Target Composition

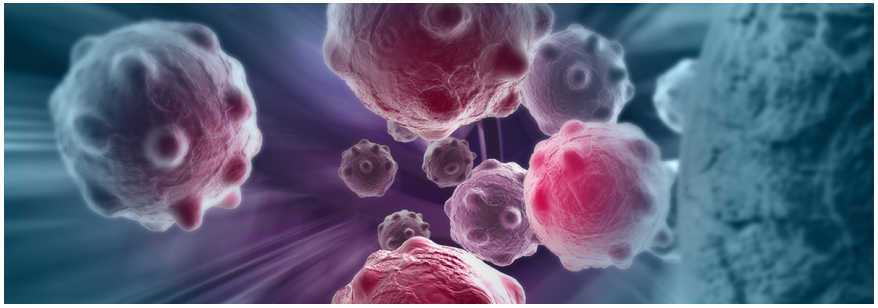


Signaling Pathways



Disease Indications





Other related Compound Libraries

Compound Library	Size	Comments
Anti-Cancer Drug Library L2150	2217	Including the most current FDA-approved anticancer drugs and compounds that have a history of use in human clinical trials; Detailed information: structure, solubility, target, activity, IC50 value, and biological activity description; Intended to enable cancer research, drug discovery and combination studies.

Other related Compound Libraries

Compound Library	Size	Comments
Clinical Compound Library L3400	2500	All compounds have a history of use in human clinical trials and known safety profiles; These compounds have known biological activities, low toxicity, and clear mechanism with demonstrated pre-clinical evidence; Every compound contains detailed information on pharmacological activities, targets, clinical development status, and indications with broad spectrum covering several therapeutic areas from cancer, inflammation, infection, neuropsychiatry to cardiology, and many drug targets such as JAK, EGFR, mTOR, CDK, HDAC, AKT, PARP, etc.
FDA-Approved Drug Library L4200	1470	1470 FDA-approved drugs with well-characterized biological activity, clear targets, safety, and bioavailability; Covers various research areas: oncology, cardiology, anti-inflammatory, immunology, neuropsychiatry, analgesia, etc.; Effective tool for drug repurposing, small molecule inducing stem cell differentiation, and target identification in mechanism interrogation.

Clinical Compound Library

Catalog No. L3400 — 2500 compounds

A Clinical Compound Library collects 2500 compounds, all of which have been permitted into the clinical trial phases. These compounds have known biological activities, low toxicity, and clear mechanism with demonstrated preclinical evidence.
Every compound contains detailed information on pharmacological activities, targets, clinical development status, and indications with broad spectrum covering several therapeutic areas from cancer, inflammation, infection, neuropsychiatry to cardiology, and many drug targets such as JAK, EGFR, mTOR, CDK, HDAC, AKT, PARP, etc. It is an effective tool for drug screening as well as cell differentiation induction.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	29,724.00
250 µL *1 0 mM (in DMSO)	USD	48,780.00
1 mg	USD	48,780.00

Drug Repurposing Compound Library

Catalog No. L9200 — 3512 compounds

Traditional de novo drug discovery and development involves an HTS campaign for de novo candidate hits and requires highly specialized screening facilities and compound libraries containing several million compounds. It is a time-consuming and expensive process. As the regulation for drug safety and efficacy is increasingly complex, the cost of developing new drugs is skyrocketing. Drug repurposing, also known as the new use of old drugs, is an effective strategy to find new indications for existing drugs. It has recently drawn attention and led to several blockbuster drugs because of its high efficiency and low-cost. High-content screenings, new biomarkers, noninvasive imaging techniques, and advances in bioinformatics have created new opportunities for pursuing novel indications for approved compounds.
The Drug Repurposing Compound Library by TargetMol®, containing 3512 approved and clinical drugs, which have undergone extensive preclinical studies and have well-characterized bioactivities, safety and bioavailability – properties that could dramatically accelerate drug development and optimization, is a good tool for drug repurposing and cell induction.
In addition, For peptides and other drug molecules with low solution stability, we provide them in the form of dry powder (set as Part B) to ensure the optimum condition of our compound library and increase the probability of successful screening.

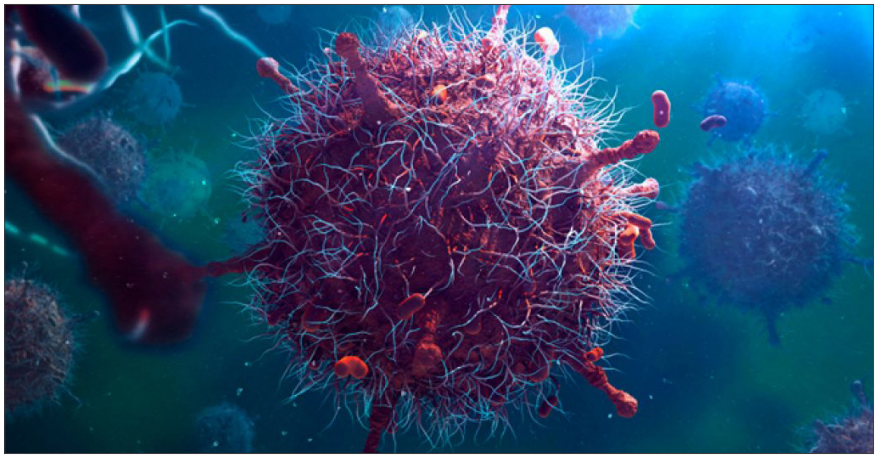
Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	28,119.00
250 µL *1 0 mM (in DMSO)	USD	49,534.00
1 mg	USD	49,534.00

FDA-Approved & Pharmacopeia Drug Library

Catalog No. L1010 — 2978 compounds

Traditional de novo drug discovery and development involves an HTS campaign for de novo candidate hits and requires highly specialized screening facilities and compound libraries containing several million compounds. It is a time-consuming and expensive process. As the regulation for drug safety and efficacy is increasingly complex, the cost of developing new drugs is skyrocketing. Drug repurposing, also known as the new use of old drugs, is an effective strategy to find new indications for existing drugs. It has recently drawn attention and led to several blockbuster drugs because of its high efficiency and low-cost. High-content screenings, new biomarkers, noninvasive imaging techniques, and advances in bioinformatics have created new opportunities for pursuing novel indications for approved compounds.
Approved drugs have known and well-characterized bioactivities, safety and bioavailability – properties that could dramatically accelerate drug development and optimization. Hits from this set will provide a significant head start in any drug optimization program. In addition, a growing number of compounds have been identified from this library that can functionally replace reprogramming transcription factors, enhance the efficiency of iPSC generation and accelerate the reprogramming process by single use or a combination of several molecules.
TargetMol®'s FDA-Approved & Pharmacopeia Drug Library collects 2978 compounds from approved institutions such as FDA, EMA, PMDA, NMPA, etc. or pharmacopoeia such as USP, BP, JP, etc., which can be used for drug repurposing and cell induction.
In addition, For peptides and other drug molecules with low solution stability, we provide them in the form of dry powder (set as Part B) in order to ensure the optimum condition of our compound library and increase the probability of successful screening.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	14,890.00
250 µL *1 0 mM (in DMSO)	USD	29,613.00
1 mg	USD	29,613.00



FDA-Approved Drug Library

Catalog No. L4200 — 1470 compounds

All compounds in FDA-Approved Drug Library have well-characterized biological activity, clear targets, safety, and bioavailability – properties that could dramatically accelerate drug development and optimization. It is an effective and ideal tool for drug repurposing and cell differentiation induction. Detailed information on each compound in this library can help scientists quickly finish drug screening or make a quick judgement on cell differentiation mechanism, and create conditions for further investigation on the mechanism of action.
In addition, For peptides and other drug molecules with low solution stability, we provide them in the form of dry powder (set as Part B) in order to ensure the optimum condition of our compound library and increase the probability of successful screening.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	8,350.00
250 µL *1 0 mM (in DMSO)	USD	15,448.00
1 mg	USD	15,448.00

Preclinical Compound Library

Catalog No. L3410 — 619 compounds

Preclinical Compound Library is a collection of 619 compounds that are in preclinical phase with clear targets and detailed information on disease indication and reference.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	8,666.00
250 µL *1 0 mM (in DMSO)	USD	12,380.00
1 mg	USD	12,380.00

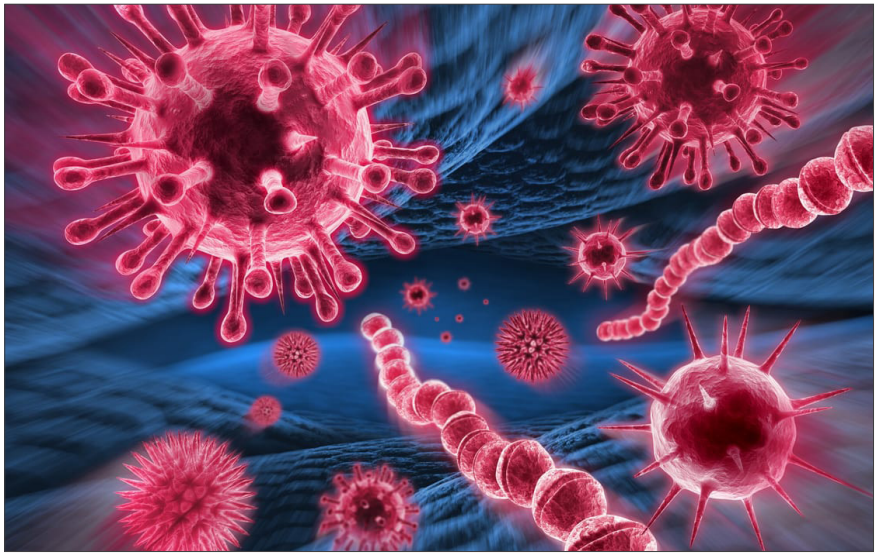
COVID-19-related Compound Libraries

3CLpro-Targeted Compound Library (CADD)

Catalog No. L1712 — 161 compounds

The 3CLpro (Mpro), also known as Nsp5, is first automatically cleaved from poly-proteins to produce mature enzymes, and then further cleaves downstream Nsps at 11 sites to release Nsp4–Nsp1631. 3CLpro directly mediates the maturation of Nsps, which is essential in the life cycle of the virus. The detailed investigation on the structure and catalytic mechanism of 3CLpro makes 3CLpro an attractive target for anti-coronavirus drug development. Inhibitors targeting at SARS-CoV 3CLpro mainly include peptide inhibitors and small-molecule inhibitors.
Based on the protein structure of 3CLpro, we selected 161 top-ranked docked molecules into 3CLpro-Targeted Compound Library (CADD) by molecular docking virtual screening against 15,376 compound structures. To speed up the research and development of anti-SARS-CoV-2 drugs, we provide the results of virtual screening for free!

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	2,660.00



ACE2-Targeted Compound Library (CADD)

Catalog No. L1713 — 462 compounds

The host ACE2 has been proved by many studies to be the specific receptor for the Spike RBD of SARS-CoV-12. The latest research shows that the host receptor of SARS-CoV-2 is consistent with SARS-CoV, indicating that the Spike RBD sequence of SARS-CoV-2 is similar to SARS-CoV RBD where important interactions exist between several key amino acid residues of RBD receptor-binding motif and ACE2. Based on the current research progress, ACE2 is considered as a host target for the treatment of coronavirus infection to block SARS-CoV-2 from entering host cells.
By binding with ACE2, small molecules have the potential to disrupt the interaction of ACE2 with RBD. Based on the protein structure of human ACE2, we selected 462 top-ranked docked molecules for ACE2-Targeted Compound Library (CADD) using molecular docking virtual screening against 15,376 compound structures. To speed up the research and development of anti-SARS-CoV-2 drugs, we provide the results of virtual screening for free!

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	6,600.00

Anti-COVID-19 Compound Library

Catalog No. L1710 — 2448 compounds

In response to the outbreak of COVID-19 caused by a novel coronavirus SARS-CoV-2, global scientific research institutions and pharmaceutical companies are stepping up related vaccine development and antiviral drug trials. Scientists from multiple countries are working hard to identify drug candidates that can be used for clinical therapy in patients with COVID-19 by screening compound libraries. TargetMol®, as a drug screening expert, quickly generated this compound library to support the research and development of anti-COVID-19 drugs.
This compound library includes Part1 and Part2. Part1 contains compounds that have been demonstrated to have an anti-coronavirus activity or are broad-spectrum antiviral agents, including Remdesivir, Lopinavir/Ritonavir, Chloroquine diphosphate (used in combination with Remdesivir), Polydatin (binds with Mpro), etc. Part2 collects compounds from virtual screening hits based on molecular docking. These compounds with high-affinity to seven SARS-CoV-2 protein targets (RBD of Spike protein, viral papain like protease (PLpro), main protease (3CLpro, also named 3-chymotrypsin-like protease), RNA-dependent RNA polymerase (RdRp), Nsp16 (2'-O-methyltransferase, helicase), Nsp15, and X-domain.) and one human ACE2 have the potential to provide more drug candidates for molecular and cellular antiviral activity assays.
As a world-renowned supplier of small molecular compounds, TargetMol® performed a Swiss-Model Homology Modelling process immediately after the outbreak of COVID-19 to generate reliable protein models or 3D protein structures of these related drugs targets. Then structure-based virtual screening was performed against TargetMol® libraries (7729 compounds) and Bioactive Compound Library (7647 compounds) using Surflex-Dock in the Sybyl-X 2.0 package. About 2000 hits having anti-COVID-19 CADD activity from virtual screening formed Part2 of this compound library. We wish these compounds would speed up the development of COVID-19 targeted drugs. We will also update it constantly in response to the latest research progress.

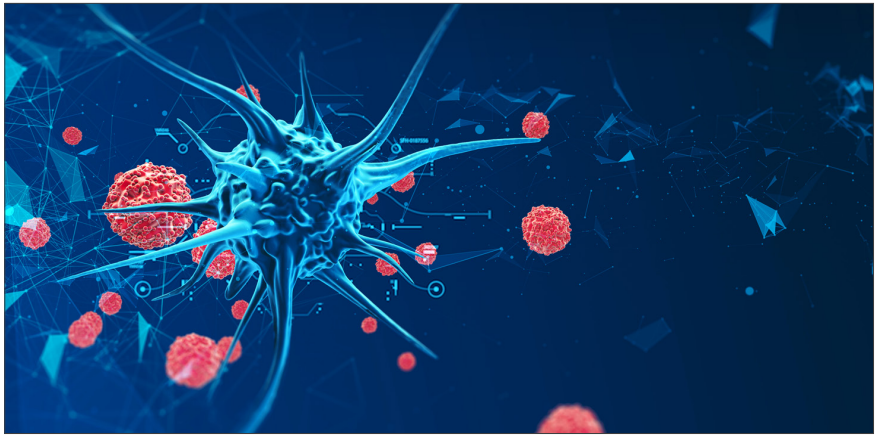
Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	23,990.00

Anti-COVID-19 Compound Library (CADD)

Catalog No. L1711 — 362 compounds

COVID-19 virus proteins are homologous to SARS-CoV proteins with an identity value ≥65%. As a world-renowned supplier of small molecular compounds, TargetMol® performed a Swiss-Model Homology Modelling process to generate reliable protein models or 3D protein structures of RBD of Spike protein, ACE2, viral papain like protease (PLpro), main protease (3CLpro, also named 3-chymotrypsin-like protease), RNA-dependent RNA polymerase (RdRp), Nsp16 (2'-O-methyltransferase, helicase), and X-domain. These 3D structures provide valuable information and foundation for structure-based virtual screening. Later, scientists from the University of Chicago published a paper titled “Crystal structure of Nsp15 endoribonuclease NendoU from SARS-CoV-2” at BioRxiv, where the high-resolution crystal structure of endoribonuclease Nsp15/NendoU from SARS-CoV-2 was reported. Studies published in 2010 on SARS-CoV revealed that inhibition of Nsp15 can slow down viral replication. This suggests drugs designed to target Nsp15 could be developed as effective drugs against COVID-19.
Molecular docking-based virtual screening can speed up the development of COVID-19-targeted drugs with high-affinity by providing more drug candidates for screening and validation at molecular and cellular levels. We used these seven virus proteins and human ACE2 as targets to screen against TargetMol® libraries (7729 compounds) and Bioactive compound library (7647 compounds) by using Surflex-Dock in the Sybyl-X 2.0 package.
To improve the virtual screening efficiency and reliability, we took a strategy of combining three rounds of screening: 2 rounds of molecular docking virtual screening plus one round of manual screening. Finally, 362 compounds were selected to form this library: Anti-COVID-19 Compound Library (CADD). These compounds have been widely reported in literatures to either have the potential of anticancer, antibacterial, anti-inflammation, anti-oxidation activity; or have other potential targets. If they were confirmed and validated in antiviral activity assay, this screening strategy, equally a novel strategy of drug repurposing or target identification of natural products, could lead to the rapid discovery of drug leads with clinical potential in response to new infectious diseases for which no prior specific drugs or vaccines are available.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	5,977.00



Nsp15-Targeted Compound Library (CADD)

Catalog No. L1719 — 470 compounds

The 3D structure of a potential drug target in a newly mapped protein of COVID-19, or coronavirus, has been solved by a team of researchers from the University of California, Riverside, the University of Chicago, the U.S. Department of Energy's Argonne National Laboratory, and Northwestern University. ("Crystal structure of Nsp15 endoribonuclease NendoU from SARS-CoV-2", BioRxiv)
In this study, the high-resolution crystal structure of endoribonuclease Nsp15/NendoU from SARS-CoV-2 was reported. The protein Nsp15 from SARS-CoV-2, is 89% identical to the protein from the earlier outbreak of SARS-CoV. Studies published in 2010 on SARS-CoV revealed that inhibition of Nsp15 can slow viral replication. This suggests drugs designed to target Nsp15 could be developed as effective drugs against COVID-19.
Based on the protein structure of Nsp15 protein, we selected 470 top-ranked docked molecules to build Nsp15-Targeted Compound Library (CADD) by molecular docking virtual screening against 15,376 compound structures. To speed up the research and development of anti-SARS-CoV-2 drugs, we provide the results of virtual screening for free!

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	7,050.00

Nsp16-Targeted Compound Library (CADD)

Catalog No. L1715 — 281 compounds

Most viral mRNAs possess a 5'-terminal cap structure (m7GpppN) essential for efficient splicing, nuclear export, translation and stability. This structure undergoes methylation catalyzed by non-structural protein 16 (Nsp16), 2'-O-ribose methyltransferase, at the ribose 2'-O position of the first and second nucleotide of the mRNA. Nsp16 provides the viral mRNA to camouflage and obscure itself from the host cell, thus preventing recognition and activation of the host immune response which is essential for successful viral infection. This protein can, therefore, act as another potential drug target for the SARS-CoV-2.
Based on the protein structure of Nsp16 protein, we selected 281 top-ranked docked molecules to build Nsp16-Targeted Compound Library (CADD) by molecular docking virtual screening against 15,376 compound structures. To speed up the research and development of anti-SARS-CoV-2 drugs, we provide results of virtual screening for free!

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	4,710.00

PLpro-Targeted Compound Library (CADD)

Catalog No. L1716 — 474 compounds

PLpro is responsible for the cleavages of N-terminus of the replicase poly-protein to release Nsp1, Nsp2 and Nsp3, which is essential for correcting virus replication. PLpro was also confirmed to be significant to antagonize the host's innate immunity. As an indispensable enzyme in the process of coronavirus replication and infection of the host, PLpro has been a popular target for coronavirus inhibitors. It is very valuable for targeting PLpro to treat coronavirus infections, but no inhibitor has been approved by the FDA for marketing.
Based on the protein structure of PLpro, we selected 474 top-ranked docked molecules to build PLpro-Targeted Compound Library (CADD) by molecular docking virtual screening against 15,376 compound structures. To speed up the research and development of anti-SARS-CoV-2 drugs, we provide the results of virtual screening for free!

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	6,750.00

RBD-Targeted Compound Library (CADD)

Catalog No. L1714 — 206 compounds

Spike is the main structural protein of coronavirus and assembles into a special corolla structure on the surface of the virus as a trimer. Spike is the main protein that interacts with the host by binding to host cell receptors to mediate virus invasion and determine viral tissue or host tropism. Spike is cleaved into S1 and S2 by the host cell protease like TMPRSS2, etc. The main function of S1 is to bind with host cell surface receptors through RBD, and the S2 subunit mediates virus–cell and cell–cell membrane fusion. Spike structural integrity and cleavage activation play a key role in virus invasion and virulence. Therapeutic strategies to block coronavirus from entering host cells by targeting RBD of Spike proteins or specific receptors on the host surface are valuable for developing antiviral drugs.
Based on the protein structure of RBD of S protein, we selected 206 top-ranked docked molecules to build RBD-Targeted Compound Library (CADD) by molecular docking virtual screening against 15,376 compound structures. To speed up the research and development of anti-SARS-CoV-2 drugs, we provide the results of virtual screening for free!

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	3,400.00

RdRP-Targeted Compound Library (CADD)

Catalog No. L1717 — 464 compounds

RdRp (Nsp12), a conserved protein in coronavirus, is an RNA-dependent RNA polymerase (RdRp) and the vital enzyme of coronavirus replication/transcription complex. The RdRp domain of polymerase is located at the C-terminus and has a conserved Ser-Asp-Asp motif. Nsp8 can de novo synthesize up to 6 nucleotides in length, which can be used as a primer for Nsp12-RdRp RNA synthesis. Further, the Nsp7_Nsp8 complex increases the binding of Nsp12 to RNA and enhances the RdRps enzyme activity of Nsp12. In the research of SARS-CoV and MERS-CoV inhibitors, Nsp12-RdRp has been used as a very important drug target. In principle, targeted inhibition of Nsp12-RdRp could not cause significant toxicity and side effects on host cells, but no specific inhibitors have been found until now.
Based on the protein structure of RdRP, we selected 464 top-ranked docked molecules to build RdRP-Targeted Compound Library (CADD) by molecular docking virtual screening against 15,376 compound structures. To speed up the research and development of anti-SARS-CoV-2 drugs, we provide the results of virtual screening for free!

Pack Size		Price
100 μL * 10 mM (in DMSO)	USD	6,600.00

X Domain-Targeted Compound Library (CADD)

Catalog No. L1718 — 463 compounds

X domain is a conserved structure of Pp1a and becomes a part of Nsp3 after Pp1a is cleaved by a virally encoded cysteine protease, the papain-like protease (PLpro). Nsp3 is a viral transmembrane domain-containing protein, a component of the replicase complex, and is of special interest since it is believed to be part of the central scaffolding protein of the replicase complex due to the large number of interactions with other Nsps. The N-terminal region of the Nsp3 (181-1000) is highly conserved among CoV, containing a ubiquitin-like (Ubl) globular fold followed by a flexible, extended acidic-domain (AC domain) rich in glutamic acid (38%). Next to the AC domain is a catalytically active ADP-ribose-1 " -phosphatase (ADRP, app-1" -pase) domain (also called macro domain or X domain) thought to play a role during the synthesis of viral subgenomic RNAs .
Based on the protein structure of The X domain, we selected 463 top-ranked docked molecules to build X Domain-Targeted Compound Library (CADD) by molecular docking virtual screening against 15,376 compound structures. To speed up the research and development of anti-SARS-CoV-2 drugs, we provide the results of virtual screening for free!

Pack Size		Price
100 μL * 10 mM (in DMSO)	USD	6,600.00

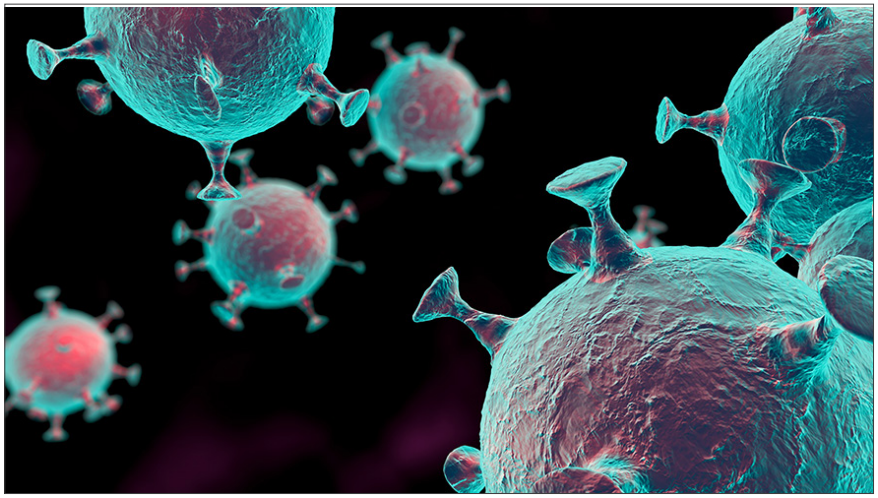
Disease-related Compound Libraries

Anti-Aging Compound Library

Catalog No. L8200 — 3050 compounds

Aging is a natural process of becoming older. The causes of aging are assigned to programmed and damage or error theories. The programmed theories imply that aging relies on specific gene regulation, and the damage or error theories emphasize the internal and environmental damages accumulated to living organisms. The damage theories proposed the nine hallmarks that were generally considered to contribute to the aging process: genomic instability, telomere attrition, epigenetic alterations, loss of proteostasis, deregulated nutrient-sensing, mitochondrial dysfunction, cellular senescence, stem cell exhaustion, and altered intercellular communication.
There is great interest in finding drugs capable of extending human lifespan and healthspan. Compounds are sought that are capable of modulating multiple aging pathways, thereby preventing a broad-spectrum of age-related diseases. The TargetMol®'s Anti-Aging Compound Library, a unique collection of 3050 anti-aging compounds, is an effective tool for anti-aging research, and anti-aging drug screening.

Pack Size		Price
100 μL * 10 mM (in DMSO)	USD	34,200.00
250 μL * 10 mM (in DMSO)	USD	56,996.00
1 mg	USD	56,996.00

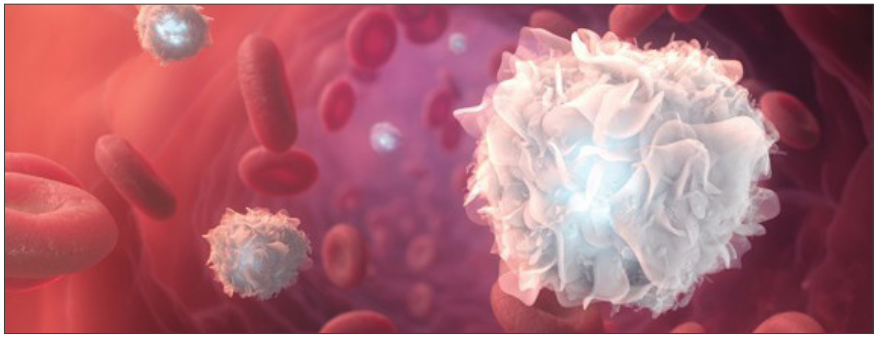


Anti-Alzheimer's Disease Compound Library

Catalog No. T002-00000002 — 650 compounds

Alzheimer's disease (AD) is a progressive neurodegenerative disease with deficits in recent memory, wordfinding, and language difficulties, and gradually progresses to global cognitive impairment. The cognitive deficits are accompanied by a variety of abnormal neurological and psychiatric symptoms that increase in frequency and severity as the disease progresses. The cause of Alzheimer's disease is unknown but the fifth-leading cause of death among those age 65 and older. The pathological features of AD mainly include cholinergic dysfunction, extracellular accumulation and deposition of Aβ peptides, intracellular neurofibrillary tangles, and other aberrant signaling pathways. Scientists have found that reducing brain Aβ levels, preventing the excessive phosphorylation of tau protein, rendering mitochondria resistant to damage, protecting neurons from apoptotic processes, controlling microglial activation, inhibiting the release of interleukin-2 and TNF-α, preventing oxidative stress damage; regulating the targets in cholinergic system, inhibiting the over activation of NMDA receptor to reduce the excitotoxicity can halt Alzheimer's disease.
Although Alzheimer's disease (AD) is the world's leading cause of dementia and the population of patients with AD continues to grow, no new therapies have been approved in more than a decade. Over the past decade, the focus of drug discovery and development efforts has shifted from symptom improving toward disease-modifying therapies for AD; that is, treatments whose aim is to affect the underlying disease process by impacting one or more of the many brain changes characteristic of AD. Many clinical trials of single-agent therapies have failed to affect disease progression or symptoms compared with placebo. The complex pathophysiology of AD may necessitate combination treatments rather than monotherapy. In addition, small molecules targeting neural stem cells (NSCs) regeneration represents a new drug discovery strategy.
TaregtMol®'s Anti-Alzheimer's Disease Compound Library, a collection of 650 compounds with anti-AD activities or acting on main drug targets of PD, can be used for related drug discovery and pharmacology research.

Pack Size		Price
100 μL * 10 mM (in DMSO)	USD	9,734.00
250 μL * 10 mM (in DMSO)	USD	17,528.00
1 mg	USD	17,528.00



Anti-Bacterial Compound Library

Catalog No. L4520 — 1074 compounds

Antibiotics are used to treat or prevent bacterial infections, and sometimes protozoan infections, having saved thousands of lives. The discovery and application of antibiotics added 5-10 years to the life expectancy of the average American. However, inappropriate antibiotic treatment and overuse of antibiotics have contributed to the emergence of antibiotic-resistant bacteria. Some strains have become resistant to practically all of the commonly available agents (multidrug resistance), one of the most important current threats to public health. Therefore, there is a critical need to develop new antimicrobials effective against these difficult-to-treat multidrug-resistant pathogens.
TargetMol®'s Anti-Bacterial Compound Library collects various antibiotics and antibacterial compounds with unique structures by fully considering the bioactivity and structure of selected compounds. This library, consisting of 1074 small molecules with antibacterial activity, is an effective tool for antibiotics and antibacterial drug development.

Pack Size		Price
100 μL * 10 mM (in DMSO)	USD	20,116.00
250 μL * 10 mM (in DMSO)	USD	34,199.00
1 mg	USD	34,199.00

Anti-Breast Cancer Compound Library

Catalog No. L2191 — 1052 compounds

Breast cancer is an uncontrolled growth of breast cells. Among women, breast cancer is the second most common cancer diagnosed, after skin cancer, and the second leading cause of cancer death, after lung cancer. In recent years, incidence rates have increased slightly (by 0.3% per year).
There are several types of breast cancer, and they are broken into two main categories: noninvasive or in situ (ductal or lobular), and invasive (ductal or lobular). In addition, breast cancer can be categorized into four molecular subtypes: a “basal-like” subgroup with low estrogen receptor (ER)/progesterone receptor (PR)/human epidermal growth factor receptor 2 (HER2) and expression of basal cytokeratins (ER-PR-HER2-); a subgroup mainly driven by HER2 amplification and overexpression while being ER/PR low (ER-PR-HER2+); a luminal A group with high ER/PR and low HER2 (ER+PR+HER2-); a luminal B group with high ER/HER2 and low PR (ER+PR-HER2+). Depending on the cancer's stage and molecular type, treatment options and prognostics of breast cancers are different: a combination of surgery, radiation therapy, chemotherapy, hormone therapy and/or administration of targeted therapy (anti-HER2) or non-HER2 targeted therapy. Several potential targets for new breast cancer drugs have been identified in recent years. Drugs based on these targets, such as kinase inhibitors (AKT), and PD-L1, are now being studied to treat triple-negative breast cancers, either by themselves, or in combination with chemotherapy.
TargetMol®'s Anti-Breast Cancer Compound Library collects 1052 compounds related to breast cancer, including all reported compounds with anti-breast cancer therapeutic effect, and compounds targeting related targets in signaling pathway (HER-2, VEGF, EGFR, PARP, CDK4/6, HSP, PD-1, SET7/9, BRCA, etc.). It is a powerful tool for breast cancer drug discovery.

Pack Size		Price
100 μL * 10 mM (in DMSO)	USD	15,655.00
250 μL * 10 mM (in DMSO)	USD	26,050.00
1 mg	USD	26,050.00

Anti-Cancer Active Compound Library

Catalog No. L2160 — 1656 compounds

During the past decades, we have witnessed many landmark discoveries and successes in cancer research and therapy, however, cancer is still a major health problem for human beings, and it often physically and emotionally brings pains and difficulties to those living with it. Cancer cells remain undifferentiated (continue to divide, to cause more damage, and invade new tissue), lack normal cell signaling responses (loss of contact inhibition and evasion of programmed cell death), contain abnormal changes (genetic abnormalities) in chromatin, have altered energy metabolism, and induce vascularization (ensure a steady supply of oxygen and nutrients).
We carefully selected 1656 compounds with known antitumor activity as Anti-Cancer Active Compound Library that can be used for tumor-related research and antitumor drug screening.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	18,994.00
250 µL * 10 mM (in DMSO)	USD	31,171.00
1 mg	USD	31,171.00

Anti-Cancer Approved Drug Library

Catalog No. L2110 — 1400 compounds

During the past decades, we have witnessed many landmark discoveries and successes in cancer research and therapy, however, cancer is still a major health problem for human beings, and it often physically and emotionally brings pains and difficulties to those living with it. Cancer cells remain undifferentiated (continue to divide, to cause more damage, and invade new tissue), lack normal cell signaling responses (loss of contact inhibition and evasion of programmed cell death), contain abnormal changes (genetic abnormalities) in chromatin, have altered energy metabolism, and induce vascularization (ensure a steady supply of oxygen and nutrients).
We carefully selected 1400 approved anticancer drugs based on published literature and database to form this collection that can be used as positive controls in biological cancer investigation and cancer correlation study.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	16,644.00
250 µL * 10 mM (in DMSO)	USD	27,315.00
1 mg	USD	27,315.00

Anti-Cancer Clinical Compound Library

Catalog No. L2120 — 1776 compounds

During the past decades, we have witnessed many landmark discoveries and successes in cancer research and therapy, however, cancer is still a major health problem for human beings, and it often physically and emotionally brings pains and difficulties to those living with it. Cancer cells remain undifferentiated (continue to divide, to cause more damage, and invade new tissue), lack normal cell signaling responses (loss of contact inhibition and evasion of programmed cell death), contain abnormal changes (genetic abnormalities) in chromatin, have altered energy metabolism, and induce vascularization (ensure a steady supply of oxygen and nutrients).
We carefully select 1776 anticancer compounds currently in clinical trial phases based on published literature and database to form this collection that can be used for high throughput screening and high content screening.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	21,115.00
250 µL * 10 mM (in DMSO)	USD	34,652.00
1 mg	USD	34,652.00

Anti-Cancer Compound Library

Catalog No. L2100 — 4730 compounds

During the past decades, we have witnessed many landmark discoveries and successes in cancer research and therapy, however, cancer is still a major health problem for human beings, and it often physically and emotionally brings pains and difficulties to those living with it. Cancer cells remain undifferentiated (continue to divide, to cause more damage, and invade new tissue), lack normal cell signaling responses (loss of contact inhibition and evasion of programmed cell death), contain abnormal changes (genetic abnormalities) in chromatin, have altered energy metabolism, and induce vascularization (ensure a steady supply of oxygen and nutrients).
We carefully selected 4730 compounds with antitumor activity based on different characteristics and abnormal metabolism with cancer cells. All of these compounds are the small molecules modulating the metabolism, growth, invasion, and metastasis of tumor cells that can be used for tumor-related research and antitumor drug screening.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	37,837.00
250 µL * 10 mM (in DMSO)	USD	65,578.00
1 mg	USD	65,578.00

Anti-Cancer Drug Library

Catalog No. L2150 — 2217 compounds

During the past decades, we have witnessed many landmark discoveries and successes in cancer research and therapy, however, cancer is still a major health problem for human beings, and it often physically and emotionally brings pains and difficulties to those living with it. Cancer cells remain undifferentiated (continue to divide, to cause more damage, and invade new tissue), lack normal cell signaling responses (loss of contact inhibition and evasion of programmed cell death), contain abnormal changes (genetic abnormalities) in chromatin, have altered energy metabolism, and induce vascularization (ensure a steady supply of oxygen and nutrients).
We carefully selected 2217 anticancer drugs including FDA approved and compounds in clinical trial phases as Anti-Cancer Drug Library that can be used for tumor-related research and antitumor drug screening.

Product Advantage

- A unique collection of 2217 anti-cancer compounds that are FDA approved or currently in clinical trial phases;
- Bioactivity and safety are confirmed by preclinical research and clinical setting, representing the cutting-edge treatments for cancers. It is a powerful tool for drug repurposing discovery and research in tumorigenesis;
- Covers various major targets including PI3K, HDAC, mTOR, CDK, Aurora Kinase, JAK, etc, involved in 15 different cancer research areas, such as lung cancer, breast cancer, leukemia, lymphoma, etc.;
- Detailed compound information with structure, target, activity, IC50 value, and brief introduction;
- NMR and HPLC/LCMS were validated to ensure high purity and quality and reduce the false-positiverate.

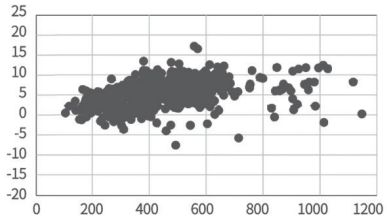
Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	26,224.00
250 µL * 10 mM (in DMSO)	USD	43,257.00
1 mg	USD	43,257.00

Drug-Like Properties

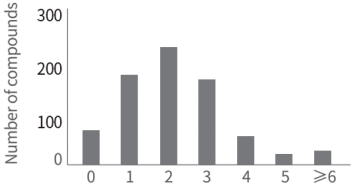
% of compounds compliant with Lipinski' s Rules

PhysChem Properties	% Compounds
<5 H-Bond donors	93
<10 H-Bond acceptors	86
cLogP<5	87
MW<500	74

cLogP vs MW

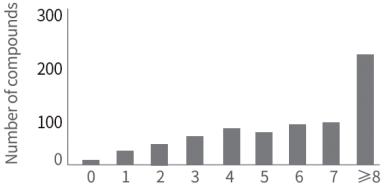


Distribution of HB Donors



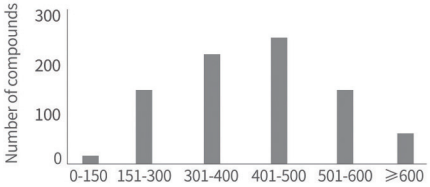
HB Donor

Distribution of HB Acceptors



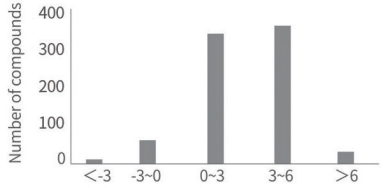
HB Acceptor

Distribution of Molecular Weight



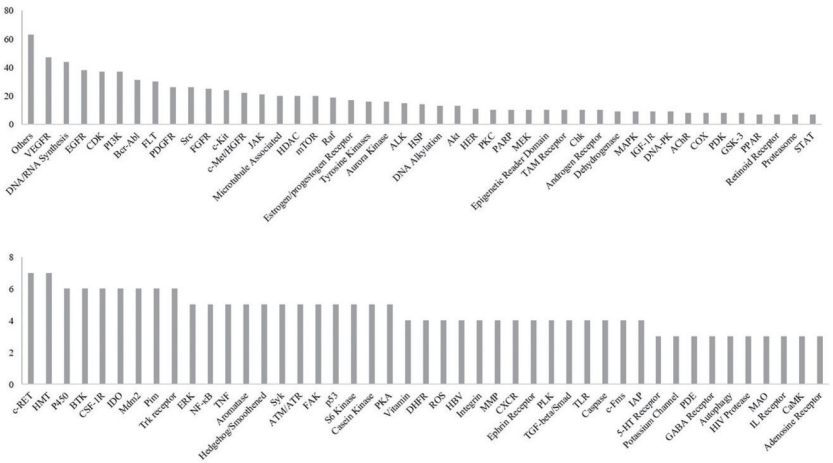
Molecular Weight

Distribution of cLogP

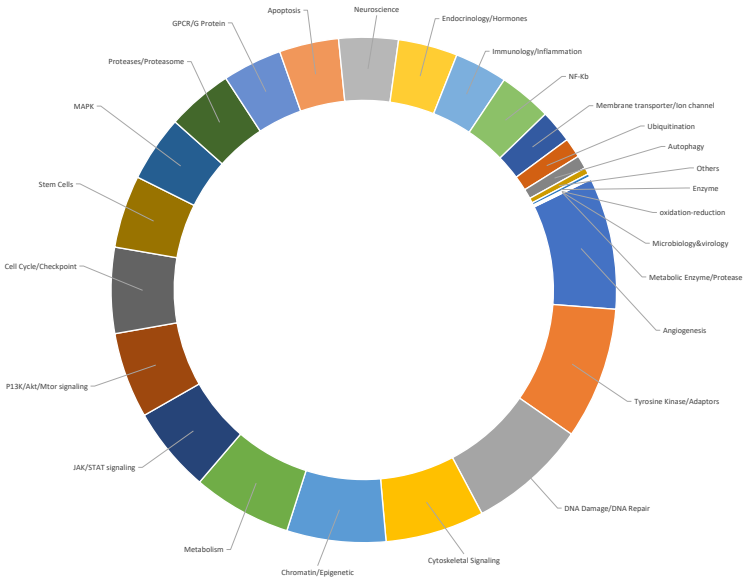


cLogP

Target Composition

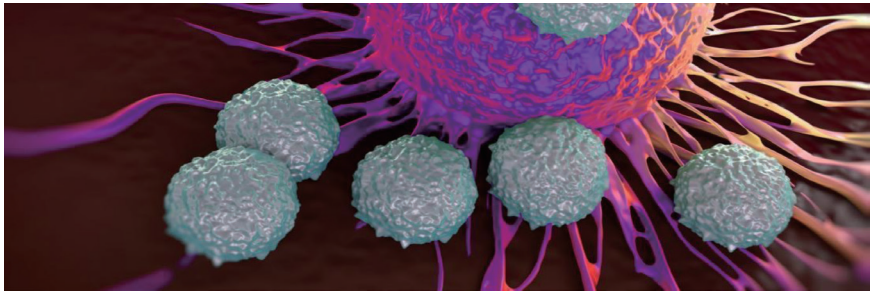


Signaling Pathways



Other related Compound Libraries

Compound Library	Size	Comments
Anti-Cancer Compound Library L2100	4730	4730 compounds with known /potential anti-cancer activity for high throughput screening (HTS) and high content screening (HCS); Effective tool for molecular mechanism of tumorigenesis, and anti-tumor drug screening; Covers various major targets including PI3K, HDAC, mTOR, CDK, Aurora Kinase, JAK, etc.
Anti-Cancer Active Compound Library L2160	1656	1656 compounds with known antitumor activity, an effective tool for molecular mechanism of tumorigenesis, and antitumor drug screening; Covers various major targets including PI3K, HDAC, mTOR, CDK, Aurora Kinase, JAK, etc. Detailed information: structure, solubility, target, activity, IC50 value, and biological activity description.
Anti-Cancer Clinical Compound Library L2120	1776	All compounds historically used in human clinical trials with known safety profiles; These compounds have known biological activities, low toxicity, and clear mechanism with demonstrated pre-clinical evidence; Every compound contains detailed information on pharmacological activities, targets, clinical development status, and indications with broad spectrum covering several therapeutic areas from cancer, inflammation, infection, neuropsychiatry to cardiology, and many drug targets such as JAK, EGFR, mTOR, CDK, HDAC, AKT, PARP, etc.
Anti-Cancer Approved Drug Library L2110	1400	1400 FDA, EMA, or CFDA approved anticancer drugs that have annotated anti-cancer activity, safety, and bioactivity; Covers various major targets including PI3K, HDAC, mTOR, CDK, Aurora Kinase, JAK, etc., in lung cancer, breast cancer, leukemia, lymphoma, etc; Effective tool for cancer research and drug repurposing screening.



Anti-Cancer Compound Library Plus

Catalog No. L2180 — 958 compounds

Cancer is a major health problem for human beings, and it often physically and emotionally brings pains and difficulties to those living with it. Cancer cells remain undifferentiated (continue to divide, to cause more damage, and invade new tissue), lack normal cell signaling responses (loss of contact inhibition and evasion of programmed cell death), contain abnormal changes (genetic abnormalities) in chromatin, have altered energy metabolism, and induce vascularization (ensure a steady supply of oxygen and nutrients). Anticancer drug development as the hottest research area has received much attention from scientists. However, in the current anticancer compound libraries, the drugs might have been discovered by different strategies or their anticancer bioactivity has been studied broadly so that the research value on them is gradually depreciated; on the other side, the application of bioactivity unknown compound library (although with a lot of unique structures) will cause lower hit rates and higher screening costs.
For this reason, TargetMol® has implemented a large-scale acquisition and testing of antitumor compounds and finally created this Anti-Cancer Compound Library Plus consisting antitumor compounds with unique structures, covering 59 tumor progression-related targets. 99% of antitumor compounds in this library, have IC50 value below 3 μM so it is a powerful tool for anticancer drug development and target identification.

Pack Size		Price
100 μL * 10 mM (in DMSO)	USD	14,282.00
250 μL * 10 mM (in DMSO)	USD	24,280.00
1 mg	USD	24,280.00

Anti-Cancer Metabolism Compound Library

Catalog No. L2130 — 1072 compounds

Cancer metabolism has emerged as an important area of research in recent years. Reprogramming of the cellular energy metabolism, essential for cancer cell proliferation and tumor development, constitutes an emerging hallmark of cancer and may serve as a biochemical basis for new therapeutic intervention. From the abnormal aerobic glycolysis effect in tumor cells was first discovered by German scientist Warburg in the early 1920s to now on all aspects of tumor metabolic activity (sugar, fat, amino acids, etc.) analysis and complex metabolic regulation network discovery, the study of tumor metabolism has entered into a more striking height. Distinct metabolic pathways (glycolysis and glutaminolysis), key regulators of aerobic glycolysis (AMPK, mTOR, HIF-1, c-Myc, p53, etc.), and key metabolism enzymes (PKM, HK, PFK, PK, IDH, GLS) might be the key targets for tumor therapeutics. Developing inhibitors targeting dysregulated metabolic enzymes and pathways may represent a promising strategy to overcome drug resistance in cancer therapy.
A unique collection of 1072 cancer cellular metabolism related compounds by TargetMol® can be used for cancer related research and high throughput and high content screening for anticancer drugs.

Pack Size		Price
100 μL * 10 mM (in DMSO)	USD	12,864.00
250 μL * 10 mM (in DMSO)	USD	21,440.00
1 mg	USD	21,440.00

Anti-Cardiovascular Disease Compound Library

Catalog No. L5400 — 987 compounds

Cardiovascular disease generally refers to all types of diseases that affect the heart or blood vessels, including coronary heart disease (clogged arteries), which can cause heart attacks, stroke, congenital heart defects and peripheral artery disease, and is the leading cause of death for men and women in the U.S. , different types of cardiovascular diseases have different mechanisms of pathogenesis. Antioxidants, lipid-lowering agents, anti-ischemic drugs, and platelet aggregation inhibitors all can reduce cardiovascular disease risk. Some natural products can inhibit the gene expression of cell adhesion molecules, cytokine, and chemokine, inhibit the function of platelet, enhance the release of nitric oxide by endothelial cells, and inhibit the contraction of smooth muscle.
A unique collection of 987 cardiovascular disease related compounds by TargetMol® can be used for cardiovascular diseases related research and high throughput and high content screening for new drugs.

Pack Size		Price
100 μL * 10 mM (in DMSO)	USD	11,768.00
250 μL * 10 mM (in DMSO)	USD	19,360.00
1 mg	USD	19,360.00

Anti-Diabetic Compound Library

Catalog No. L1900 — 468 compounds

Diabetes is a chronic, metabolic disease characterized by elevated levels of blood glucose (or blood sugar). Too much sugar in the blood for an extended period can lead to serious health problems. If left untreated, diabetes can cause many complications that would seriously impact the quality of life and shorten the life expectancy of the people with it. Currently, there is no known cure for diabetes but people with diabetes can stay healthy by managing their disease through diet and the help of medicine. A unique collection of 468 small molecules affecting the development of diabetes is an effective tool for diabetes research and drug screening.

Pack Size		Price
100 μL * 10 mM (in DMSO)	USD	7,238.00
250 μL * 10 mM (in DMSO)	USD	12,106.00
1 mg	USD	12,106.00

Anti-Fibrosis Compound Library

Catalog No. L9810 — 981 compounds

Fibrosis, also known as fibrotic scarring, is a pathological wound healing in which connective tissue replaces normal parenchymal tissue to the extent that it goes unchecked, leading to considerable tissue remodeling and the formation of permanent scar tissue. If highly progressive, the fibrotic process eventually leads to organ malfunction and death. Fibrosis affects nearly every tissue in the body, such as the lung, liver, kidney, bone marrow, etc. Fibrosis is the final, common pathological outcome of many chronic inflammatory diseases, including scleroderma, rheumatoid arthritis, Crohn's disease, ulcerative colitis, myelofibrosis and systemic lupus erythematosus.
TargetMol®'s Anti-Fibrosis Compound Library collects 981 potential anti-fibrosis compounds, including inhibitors to TGF-beta, TNF-alpha, MMP, etc., antioxidants, anti-inflammatory compounds, etc. It is a powerful tool for research in fibrosis and related drug development.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	14,598.00
250 µL * 10 mM (in DMSO)	USD	24,291.00
1 mg	USD	24,291.00

Anti-Fungal Compound Library

Catalog No. L4500 — 157 compounds

Invasive fungal infections are a significant health problem in immunocompromised patients. However, the number of therapeutic options for the treatment of invasive fungal infections is quite limited, and includes only three structural classes of drugs: polyenes, azoles, and echinocandins. Anti-Fungal Compound Library from TargetMol® is a unique collection of 157 compounds that include the natural product (polyene and echinocandins), target specific chemicals (azoles) and FDA approved antifungal agents. More recently, interest in natural product-based screening has enjoyed a renaissance. This has been driven not only by the recognition of the valuable features of natural product hits and that natural substances have evolved over a very long selection process to form optimal interactions with biological macromolecules, but by improvements in structure-identification, separation, and target identification. Recently, broad interest in combination screening to identify molecules that synergize with existing classes of antibacterial and antifungal drugs as an approach to improve efficacy has emerged. Our Anti-Fungal Compound Library is an effective tool for drug repurposing and combination screening.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	37,837.00
250 µL * 10 mM (in DMSO)	USD	65,578.00
1 mg	USD	65,578.00

Anti-Gastroenteritis Natural Product Library

Catalog No. L6600 — 112 compounds

Gastroenteritis is inflammation of the stomach lining and small and large intestines. Most cases are infectious, although gastroenteritis may occur after ingestion of drugs and chemical toxins (eg, metals, plant substances). In the US, an estimated 1 in 6 people contracts foodborne illness each year. Worldwide, an estimated 1.5 million children die each year from infectious gastroenteritis.
Compounds derived from natural products have demonstrated their effectiveness as therapeutic agents in different areas, such as cancer, aging, metabolic disorder, cardiovascular disease (controlling blood sugar), inflammation (gastroprotective effect), and neurologic disorders, etc. The gastrointestinal tract is where the natural products exert their bioactivities, such as modulating the movement of the gastrointestinal tract, protecting stomach mucosa, keeping gut bacteria in balance, and interacting with the intestinal immune system. Understanding the effects of natural products on gastrointestinal function is of significance to the treatment of related gastrointestinal diseases and drug screening.
Anti-Gastroenteritis Natural Product Library by TargetMol® is a unique collection of 112 natural products related to gastroenteritis, an effective tool for research in gastric function and related diseases, drug screening.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	1,855.00
250 µL * 10 mM (in DMSO)	USD	3,100.00
1 mg	USD	3,100.00

Anti-Hypertension Compound Library

Catalog No. L7110 — 524 compounds

Hypertension (hypertension) is a clinical syndrome characterized by increased arterial blood pressure (systolic and/or diastolic) in the body circulation (systolic blood pressure ⩾ 140 mm Hg and diastolic blood pressure ⩾ 90 mm Hg), often accompanied by clinical syndromes including metabolic disorders of fat and glucose, functional or organic changes in the heart, brain, kidney, and retina. Hypertension is the most common chronic disease and is the most important risk factor for cardiovascular and cerebrovascular diseases. The results of several studies suggest that intervention of blood pressure, early prevention and treatment of hypertension can help reduce the risk of cardiovascular disease.
TargetMol® Anti-hypertension Compound Library is a collection of 524 hypertension-related small molecules, including compounds with Anti-hypertension effects and compounds that act on hypertension-related targets, that support your research or related drug screening.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	8,522.00
250 µL * 10 mM (in DMSO)	USD	16,687.00
1 mg	USD	16,687.00

Anti-Infection Compound Library

Catalog No. L1800 — 1326 compounds

An infection happens when a foreign organism enters a person's body and causes harm. These infectious organisms are known as pathogens. Examples of pathogens include bacteria, viruses, fungi, prions, and parasites. Some infections are mild and barely noticeable, but others are severe and life-threatening, and some are resistant to treatment.
A unique collection of 1326 small bioactive molecules with antibacterial, antiviral, and antiparasitic capability was carefully selected by TargetMol® for high throughput drug screening and new drug target identification in anti-infection research.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	12,166.00
250 µL * 10 mM (in DMSO)	USD	20,284.00
1 mg	USD	20,284.00

Anti-Lung Cancer Compound Library

Catalog No. L2190 — 704 compounds

According to Global cancer statistics 2018, the global cancer burden is estimated to have risen to 18.1 million new cases and 9.6 million deaths in 2018. Nearly half of the new cases and more than half of the cancer deaths worldwide in 2018 are estimated to occur in Asia. Cancer of the lung is responsible for both the leading type of new cases (11.6% of the total cancer incidence) and the most significant number of deaths (1.8 million deaths, 18.4% of the total) worldwide because of the poor prognosis for this cancer due to lack of effective therapy.
Treatment options for lung cancer include surgery, radiation therapy, chemotherapy, immunotherapy, targeted therapy and combination therapy. Therapeutic-modalities recommendations depend on several factors, including the type and stage of cancer. Despite the improvements in diagnosis and therapy made during the past 30 years, the prognosis for patients with lung cancer is still unsatisfactory. The responses to current standard therapies are poor except for the most localized cancers.
Targeted therapy and immunotherapy have changed the treatment paradigm of non-small cell lung cancer (NSCLC) and become the future direction for lung cancer therapy based on the major advances achieved recently. Targeted therapies focus on cancer cells by interrupting their growth and how they function and help reduce damage to healthy cells. However, while targeted therapy in NSCLC has provided disease control, the tumors inevitably develop drug resistance. With the advent of whole genome sequencing technology, we will have more understanding of the biological mechanism of the occurrence and development of NSCLC and the mechanism of drug resistance thus new generation of targeted therapy overcoming drug resistance can be designed and developed.
TargetMol®'s Anti-Lung Cancer Compound Library collects 704 compounds targeting lung cancer's major signaling pathways or having anti-lung cancer therapeutic activity reported in the literature.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	11,668.00
250 µL * 10 mM (in DMSO)	USD	19,342.00
1 mg	USD	19,342.00

Anti-Metabolism Disease Compound Library

Catalog No. L5200 — 1471 compounds

Metabolism is the set of life-sustaining chemical reactions involved in maintaining the living state of the cells and the organism, including catabolism and anabolism, and is one way the body maintains homeostasis. The main focus in the metabolism research area is the biological regulatory mechanism and its role in obesity, diabetes, cardiovascular diseases, and cancer. The unique collection of 1471 small chemicals targeting metabolism diseases will provide support for metabolism research and related drug screening.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	17,400.00
250 µL * 10 mM (in DMSO)	USD	29,000.00
1 mg	USD	29,000.00

Anti-Obesity Compound Library

Catalog No. L7100 —1176 compounds

Obesity has become the public health issue of the day—for certain reasons. The data outline a dismal picture and a more foreboding future. The prevalence of obesity has doubled in adults and children and tripled in adolescents over the past 2 decades. Two-thirds of Americans are overweight or obese. Each year in the United States, 400 000 deaths and $117 billion in health-care and related costs are attributable to obesity. Obesity is a complex, multifactorial disease that develops from the interaction of genetic, social, behavioral, cultural, physiological, and metabolic factors. It is intimately linked to heart disease, sleep apnea, and certain cancers. Current main options for treatments of obesity including diet, physical exercise, behavioral therapy, and bariatric surgery have some degree of risk. Therefore, there is a strong need to develop a new effective and safe antiobesity drug. Many pharmaceutical companies have invested substantial capital and labor to develop antiobesity drugs; however, most of the antiobesity drugs that have thus far been approved and marketed have ultimately been withdrawn because of their serious adverse effects. Scientists are trying to find and identify safe and effective antiobesity bioactive ingredients from food or drugs, especially by inhibiting intestinal fat absorption, increasing fat cell metabolism, and enhancing energy expenditure, such as lipase inhibitors, alpha-glucosidase inhibitors (αGI), and Maltase - glucoamylase (MGA) inhibitors.
Traditional pharmacological monotherapies for obesity, although initially successful in achieving weight loss, are often subject to counter-regulation. This is not surprising given the multiplicity and redundancy of mechanisms involved in appetite regulation and energy homeostasis. It is therefore pertinent to note that combination agents that are designed to simultaneously target more than one biological mechanism might ultimately be more effective in producing sustained weight loss and improvements in comorbidities.
Based on the published literature, TargetMol® carefully collects 1176 compounds with antiobesity activity as Anti-Obesity Compound Library, which can be used for antiobesity research and drug discovery.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	17,507.00
250 µL * 10 mM (in DMSO)	USD	29,127.00
1 mg	USD	29,127.00

Anti-Pancreatic Cancer Compound Library

Catalog No. L2192 — 1162 compounds

With advances in early detection and cancer treatment over the past decade, such as immunotherapy, we see accelerated drops in the mortality rate of lung cancer and melanoma, as well as long-term drops in death rates of colorectal, breast, and prostate cancer. While survival rates for other cancers have increased in the last 40 years, only 7% - 10% of people with pancreatic cancer currently survive for 5 years or longer. This type of cancer with the highest mortality rate of all major cancers is often detected late, spreads rapidly, and has a poor prognosis. A lack of ways to diagnose this cancer early and the largely asymptomatic nature of the disease means that most people are diagnosed at an advanced stage when treatments such as chemotherapy are not as effective.
To meet the needs of pancreatic cancer researchers and support the pancreatic cancer drug development, TargetMol® collects 1162 compounds related to pancreatic cancer, targeting KRas, MEK, ERK, RAF, PI3K, HER2, EGFR, JAK/STAT, IGF-1R, VEGF, TGFβ, etc.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	17,291.00
250 µL * 10 mM (in DMSO)	USD	28,772.00
1 mg	USD	28,772.00

Anti-Parasitic Compound Library

Catalog No. L4510 — 358 compounds

A Parasitic disease, also known as parasitosis, is an infectious disease caused or transmitted by a parasite. Parasitic infections are distributed virtually throughout the world, with high prevalence rates in undeveloped countries and regions. Parasitic diseases such as malaria, schistosomiasis, leishmaniasis, sleeping sickness and Chagas disease affect millions of people every year, leading to severe morbidity and death. However, there has been an increasing drug resistance to antiparasitic drugs. There is a pressing need for new treatments targeting these diseases, which have often been neglected because they overwhelmingly or exclusively affect the inhabitants of developing countries.
TargetMol® collects 358 unique antiparasitic bioactive small molecules as an Anti-Parasitic Compound Library, which most are anti-malaria compounds, and some are antitrypanosomal, antischistosomal, or anti-cryptosporidial compounds with IC50s below 0.9 µM. It is a must-have screening tool for anti-parasitic drug development.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	5,337.00
250 µL * 10 mM (in DMSO)	USD	9,073.00
1 mg	USD	9,073.00

Anti-Parkinson's Disease Compound Library

Catalog No. T002-00000003 — 184 compounds

Parkinson's disease (PD), the most common neurodegenerative movement disorder, is characterized by an extensive and progressive loss of dopaminergic neurons in the substantia nigra pars compacta. The incidence of PD is 1% of the population over the age of 60. This increases to 5% of the population over age 85. This makes aging the biggest risk factor for developing PD. Parkinson’ s disease symptoms include muscle rigidity, tremors, and changes in speech and gait. PD also had more severe insomnia and more symptoms of depression. The cause of PD is not known, but a number of genetic risk factors have now been characterized, as well as several genes which cause rare familial forms of PD. Environmental influences such as smoking, caffeine consumption, and pesticide exposure have been postulated to alter the risk of PD development, although the role of these remains unclear. PD is a multifactorial disease, with both genetic and environmental factors playing a role. Currently, PD cannot be cured. Treatment predominantly focuses on symptomatic relief with drugs aiming to either restore the level of dopamine in the striatum or to act on striatal post-synaptic dopamine receptors, but none has yet been shown to slow the progression of the disease in humans.
Available drugs for PD include Levodopa, monoamine oxidase inhibitors (MAOIs), dopamine agonists, Glutamate antagonist, the putative N-methyl-o-aspartate (NMDA) receptor antagonists, COMT inhibitors, Anticholinergics, and the muscarinic receptor blockers, etc.
TargetMol®'s Anti-Parkinson's Disease Compound Library, containing 184 compounds with anti-PD activities or acting on main drug targets of PD, can be used for related drug discovery and pharmacology research.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	2,965.00
250 µL * 10 mM (in DMSO)	USD	4,957.00
1 mg	USD	4,957.00

Anti-Viral Compound Library

Catalog No. L1700 — 681 compounds

A virus is a small infectious agent that replicates only inside the living cells of other organisms through various pathways, and causes damage to the host cells. Common diseases caused by viruses include smallpox, the common cold, chickenpox, influenza, shingles, yellow fever, herpes, etc. AIDS, polio, and Ebola are examples of life-threatening serious viral diseases caused by HIV, poliovirus, and Ebola virus, respectively.
The Anti-Viral Compound Library from TargetMol® contains 681 compounds with antiviral bioactivity, and is an appropriate tool for drug repurposing for new antiviral drug discovery based on the fact that these viruses rely on common host cellular mechanisms to promote discrete stages of their life cycles.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	7,238.00
250 µL * 10 mM (in DMSO)	USD	12,106.00
1 mg	USD	12,106.00

Hematonosis Compound Library

Catalog No. L8400 — 126 compounds

Hematologic diseases (hematonosis), disorders of the blood and blood-forming organs, afflict millions of Americans. In addition to hematological malignancies, such as leukemia and lymphomas, children and adolescents can suffer from blood disorders, that are not classified as cancer, but may lead to severe diseases and therefore require treatment. These blood disorders include severe aplastic anemia (SAA), thalassemia, immune (idiopathic) thrombocytopenic purpura, congenital neutropenia, hemophilia, sickle-cell disease, iron deficiency anemia and various other diseases. In the past, due to the lack of effective treatments, many diseases have been called "incurable diseases". In recent years, with in-depth development of medical research, the treatment of blood diseases has been significantly improved. Modern medicine uses hormones, chemotherapy and other methods for the treatment of blood diseases, but the side effects are large, and the patient has a low cure rate and is prone to recurrence. Bone marrow transplantation for the treatment of leukemia was introduced then the cure rate of leukemia was improved. However, the bone marrow resources were very scarce, and a large part of the donated bone marrow was inconsistent with the patient's HLA, even if the transplant was successful, and the recurrence rate was as high as 70% within 5 years. Therefore, it is necessary to develop new therapies and drugs for the treatment of hematologic diseases.
Hematonosis Compound Library from TargetMol® provides you with compounds related to hematologic diseases that can be used for high throughput and high content screening.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	1,890.00
250 µL * 10 mM (in DMSO)	USD	3,276.00
1 mg	USD	3,276.00

Immunology/Inflammation Compound Library

Catalog No. L4700 — 2769 compounds

An autoimmune disorder occurs when the body's immune system attacks and destroys healthy body tissue by mistake. Areas often affected by autoimmune disorders include blood vessels, connective tissues, joints, and skin, etc. The chemical advances in the 19th–20th centuries brought about the development of nonsteroidal anti-inflammatory drugs (NSAIDs). Although effective in the treatment of inflammatory diseases, NSAIDs have some undesirable and adverse effects, such as ulcers, kidney injury, and bleeding in the gastrointestinal tract. Although initially identified as antitumor molecule, TNF is now considered as a pleiotropic cytokine that plays a major role in immune or inflammatory responses. Consequently, anti-TNF biologics, which are designed to block the biological function of TNF, have been developed for the therapy of autoimmune inflammatory diseases. The success of biologics for autoimmune diseases coupled with rapid advances in basic research has validated many immunology-relevant signaling pathways and uncovered new intracellular molecules to target potential new drug agents that can enter the cell. For example, many small chemicals or macrolide derivatives that can inhibit immunoproteasome, nucleus output proteins, NF-kB, and TNF-alpha have the potential to be developed as the drugs to treat autoimmune inflammatory diseases and chronic inflammatory diseases.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	27,014.00
250 µL * 10 mM (in DMSO)	USD	45,103.00
1 mg	USD	45,103.00

Anti-Nervous System Disease Library

Catalog No. L4660 — 935 compounds

The nervous system is the most complex part of the human body, regulating various life processes. However, we have very limited knowledge about the nervous system. The last decade has seen huge advances in our knowledge of the molecular, cellular and systematic signaling pathways within the nervous system. There have been significant breakthroughs in studies on the signaling pathways that underlie neurogenesis, addiction and autism spectrum disorders, as well as the pathophysiology and treatment of mood disorders, and all these will drive the breakthroughs in neurological therapeutics and patient care.
TargetMol®'s Anti-Nervous System Disease Library collects 935 small molecules with unique structures targeting nervous system disease, covering 52 nervous system disease-related targets with IC50 below 3.5 µM，is a powerful tool for drug development in nervous system disease and related studies.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	13,939.00
250 µL * 10 mM (in DMSO)	USD	23,697.00
1 mg	USD	23,697.00

Anti-Neurodegenerative Disease Compound Library

Catalog No. L2620 — 902 compounds

Neurodegenerative disorders, such as Alzheimer’ s disease (AD), Parkinson’ s disease (PD), Huntington’ s disease (HD), spinal muscular atrophy (SMA), and amyotrophic lateral sclerosis (ALS), are incurable and debilitating conditions characterized by progressive degeneration of specific neurons within the brains of affected individuals. Neurodegenerative diseases have become an enormous economic burden that is projected to grow significantly over the next few decades in the absence of any new therapeutic interventions.
Drugs for the central nervous system, including neurodegenerative diseases, that entered clinical development, have a considerably lower probability of reaching the marketplace (7%) than the industry average across other therapeutic areas (15%), and require a longer time for development and regulatory approval (average of 12.6 years) compared with most other diseases (e.g., 6.3 years for cardiovascular and 7.5 years for gastrointestinal indications).
In this compound library, TargetMol® collects 902 compounds related to neurodegenerative diseases having therapeutic effects or acting on neurodegenerative disease-related targets.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	14,668.00
250 µL * 10 mM (in DMSO)	USD	24,560.00
1 mg	USD	24,560.00

Nonsteroidal Anti-Inflammatory Compound Library

Catalog No. L4710 — 530 compounds

Nonsteroidal anti-inflammatory drugs (NSAIDs) are members of a nonsteroidal drug class that reduces pain, decreases fever, prevents blood clots, and in higher doses, decreases inflammation. There have been more than one hundred NSAIDs within about a thousand brand names on the market since "aspirin" was first synthesized in 1898. NSAIDs, including aspirin, indomethacin, naproxen, nabumetone, diclofenac, ibuprofen, Nimesulide, Rofecoxib, Celecoxib, etc., act by inhibiting COX, thereby reducing prostaglandin formation, and have been largely applied to treat osteoarthritis, rheumatoid arthritis, and tendonitis and used to reduce fever or relieve minor aches caused by the common cold.
TargetMol®'s Nonsteroidal Anti-Inflammatory Compound Library collects 530 nonsteroidal anti-inflammatory related compounds that can be used for anti-inflammatory related pharmacological studies and drug development.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	6,319.00
250 µL * 10 mM (in DMSO)	USD	10,396.00
1 mg	USD	10,396.00

Cancer Cell Differentiation Compound Library

Catalog No. L2140 — 251 compounds

Cell differentiation is a multifaceted process that depends on complex regulatory networks that involve transcriptional, post-transcriptional and epigenetic regulation of gene expression. In cancer, this describes how much or how little tumor tissue looks like the normal tissue it came from. Well-differentiated cancer cells look more like normal cells and tend to grow and spread more slowly than poorly differentiated or undifferentiated cancer cells. Differentiation is used in tumor grading systems, which are different for each type of cancer.
In addition to apoptosis resistance and cell proliferation capacities, the undifferentiated state also characterizes most cancer cells, especially leukemia cells. The induction of cancer cell differentiation is considered an alternative approach to elicit cell death and proliferation arrest. Differentiation therapy has mainly been developed to treat acute myeloid leukemia, notably with all-trans retinoic acid (ATRA). Numerous molecules from diverse natural or synthetic origins are effective alone or in association with ATRA in both in vitro and in vivo experiments. During the last two decades, pharmaceuticals and natural compounds with various chemical structures, including alkaloids, flavonoids and polyphenols, were identified as potential differentiating agents of hematopoietic pathways and osteogenesis.
TargetMol® collects 251 reported compounds inducing cancer cell differentiation as Cancer Cell Differentiation Compound Library, which can be used for high throughput and high content screening for drug discovery.

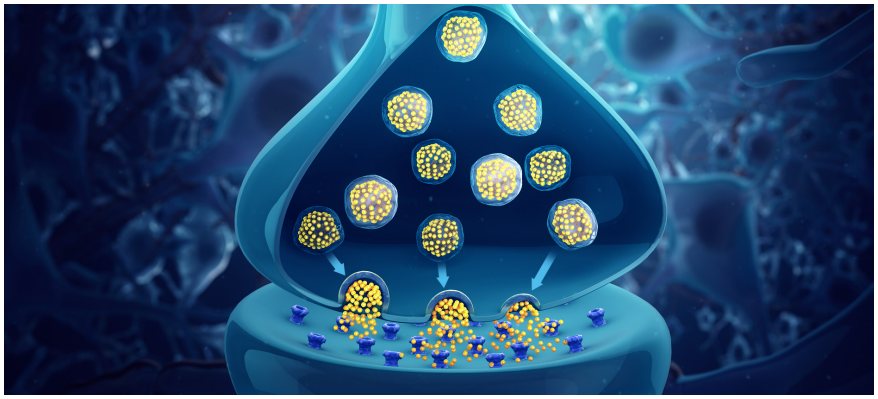
Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	3,050.00
250 µL * 10 mM (in DMSO)	USD	5,360.00
1 mg	USD	5,360.00

Immuno-Oncology Compound Library

Catalog No. L2170 — 340 compounds

Traditional cancer therapies include surgery, radiation therapy, and chemotherapy. With the rapid development of science and technology in medicine, new cancer therapies such as immunotherapy, targeted therapy, radiofrequency ablation for cancer are actively developed to help patients fight cancer. Cancer immunotherapy, also known as immuno-oncology, is a form of cancer treatment that uses the power of the body's own immune system to prevent, control, and eliminate cancer. Science magazine—America's leading scientific journal—has deemed cancer immunotherapy the 2013 “Breakthrough of the Year,” beating out nine other contenders.
There are several types of immunotherapy, including: Non-specific immunotherapies, CAR T-cell therapy, cancer vaccines, checkpoint inhibitors, etc. Most cancer immunotherapy agents being developed or approved are engineered T cells targeting tumors or mostly antibody-based biologics that target the immune checkpoint cascade. The success of these biologics in the clinic is now inspiring the discovery and development of small molecules that act on intracellular targets affecting immuno-modulatory pathways in cancer. Small molecule agents as opposed to biologics that steer or enable the immune system to attack cancer cells, represent an emerging area of R&D focus in the oncology drug development industry. Small molecules are being investigated as stand-alone agents and synergistically with approved biologics because of the ability of small molecules to reach intracellular targets and the greater patient convenience offered by their oral bioavailability. The foundation for the pursuit of small molecule immune therapies for cancer is the wide spectrum of cells and their molecular pathways that are used by the immune system to suppress or enhance cellular immunity. Such novel immunotherapeutic approaches can either negate immune suppression in the tumor milieu or facilitate cytolytic lymphocyte responses to the tumor.
TargetMol®'s Immuno-Oncology Compound Library carefully collects 340 bioactive compounds targeting intracellular pathways modulating the innate and adaptive immune response is a powerful tool for your research and drug discovery.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	7,089.00
250 µL * 10 mM (in DMSO)	USD	11,733.00
1 mg	USD	11,733.00



Library Categories based on Targets in Signaling Pathway

Adrenergic Receptor-Targeted Compound Library

Catalog No. L2700 — 117 compounds

The adrenergic receptors or adrenoceptors are a class of G protein-coupled receptors that are targets of many catecholamines like norepinephrine(noradrenaline) and epinephrine(adrenaline) produced by the body, modulating cardiovascular. A unique collection of 117 bioactive compounds by TargetMol® includes blockers, agonists, endogenous neuron transmitters, and approved drugs, and is an effective tool for screening or identifying recombinant orphan G-protein coupled receptors, new target identification, second screening, and other pharmacological applications.

Pack Size		Price
100 μL * 10 mM (in DMSO)	USD	1,938.00
250 μL * 10 mM (in DMSO)	USD	3,239.00
1 mg	USD	3,239.00

AMPK-Targeted Compound Library

Catalog No. L1120 — 36 compounds

AMPK（Adenosine 5‘-monophosphate (AMP)-activated protein kinase） plays a major role in regulating cellular energy balance by sensing and responding to increases in AMP/ADP concentration relative to ATP. Binding of AMP causes allosteric activation of the enzyme and binding of either AMP or ADP promotes and maintains the phosphorylation of threonine 172 within the activation loop of the kinase. AMP-activated protein kinase (AMPK) AMPK has attracted widespread interest as a potential therapeutic target for metabolic diseases including type 2 diabetes and, more recently, cancer.
AMPK activity is prominent in regulation of glucose, lipid, and proteins metabolism as well as mitochondrial biogenesis and autophagy. Activation of AMPK in the liver decrease blood glucose and in skeletal muscles stimulates glucose uptake independently of insulin through modulation of activity of several downstream substrates. Activation of AMPK inhibits synthesis and induces oxidation of fatty acids, which may reduce ectopic lipid accumulation and improve insulin action. The enzyme activation promotes cardiovascular homeostasis by ensuring optimum redox balance of heart and vascular tissue. In addition, AMPK signaling may link to cancer development via regulation of checkpoints of cell cycle.
TargetMol’s AMPK-Targeted Compound Library containing 36 compounds targeting AMPK can be used for research in AMPK signaling pathway and its dysfunction-related diseases.

Pack Size		Price
100 μL * 10 mM (in DMSO)	USD	738.00
250 μL * 10 mM (in DMSO)	USD	1,107.00
1 mg	USD	1,107.00

Angiogenesis Compound Library

Catalog No. L4800 — 504 compounds

Angiogenesis is a normal and vital process in growth and development, as well as in wound healing and in the formation of granulation tissue. However, uncontrolled angiogenesis underlies many deadly and debilitating conditions, including cancer, skin diseases, immune disorders, diabetic ulcers, cardiovascular disease, stroke, critical limb ischemia, and many others. Therefore, angiogenesis has become an attractive target for combating diseases characterized by either poor vascularization or abnormal vasculature. For example, angiogenesis plays a critical role in the growth of cancer. Tumors induce blood vessel growth (angiogenesis) by secreting various growth factors (e.g. VEGF) and proteins which induce capillary growth into the tumor, providing it with oxygen and nutrients. Angiogenesis is also required for the spread of a tumor, or metastasis. Therefore, angiogenesis inhibitors can be used to treat cancer. In addition, proangiogenic therapies are being explored as options to treat ischemic cardiovascular diseases by the formation of “natural bypasses” —that is, collateral vessels.
The TargetMol®'s Angiogenesis Compound Library, a unique collection of angiogenesis-related compounds, can be used for research in angiogenesis and related drug discovery.

Pack Size		Price
100 μL * 10 mM (in DMSO)	USD	12,180.00
250 μL * 10 mM (in DMSO)	USD	18,152.00
1 mg	USD	18,152.00

Apoptosis Compound Library

Catalog No. L9000 — 1383 compounds

Apoptosis is a form of programmed cell death that occurs in multicellular organisms. In contrast to necrosis, which is a form of traumatic cell death that results from acute cellular injury, apoptosis is a highly regulated and controlled process that confers advantages during an organism's lifecycle. Apoptosis leads to characteristic cell changes (morphology): the cell breaks apart into multiple vesicles called apoptotic bodies, which undergo phagocytosis. Apoptosis is regulated by both pro-apoptotic (such as Fas receptor and caspases) and anti-apoptotic (such as Bcl-2 and IAP) factors. Disordered apoptosis is implicated in a variety of human diseases. Inhibition of apoptosis can result in a number of cancers, autoimmune diseases, inflammatory diseases, and viral infections. Excessive apoptosis may also be a feature of some conditions such as autoimmune diseases, neurodegenerative diseases, and ischemia-associated injury. Consequently, considerable interest has arisen in therapeutic strategies for cancer, autoimmune diseases, and neurodegenerative diseases by modulating apoptosis pharmacologically.
TargetMol®'s collection of 1383 apoptosis-related compounds, Apoptosis Compound Library, is divided accordingly with compounds designed for either pro- or anti-apoptosis purposes and can be used for research in cancer and neurodegenerative diseases.

Pack Size		Price
100 μL * 10 mM (in DMSO)	USD	20,583.00
250 μL * 10 mM (in DMSO)	USD	34,553.00
1 mg	USD	34,553.00

Autophagy Compound Library

Catalog No. L3200 — 1067 compounds

Autophagy is the natural, regulated mechanism of the cell that disassembles unnecessary or dysfunctional components. Targeted damaged cytoplasmic constituents are isolated from the rest of the cell within a double-membrane vesicle known as an autophagosome. The autophagosome eventually fuses with lysosomes and the contents are degraded and recycled. Autophagy, cellular senescence, and apoptosis are three key responses of a cell facing stress, correlating with each other. It has been reported that defects of autophagy are associated with genomic damage, metabolic stress, and tumorigenesis. The Autophagy Compound library by TargetMol® contains 1067 compounds with defined autophagy-inducing or -inhibitory activity, and is a useful tool for studying the roles of pro- and anti-autophagic molecules in cells as well as for use in in-vitro applications.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	11,792.00
250 µL * 10 mM (in DMSO)	USD	20,052.00
1 mg	USD	20,052.00

Calcium Antagonist Library

Catalog No. L7200 — 75 compounds

A calcium channel is an ion channel(plasma membrane protein) that shows selective permeability to calcium ions. Calcium channels constitute a large family of voltage- and ligand-operated ion channels. Calcium channels are ubiquitous, they can be found in almost any type of excitable (e.g., muscle, glial cells, neurons, etc.) and most unexcitable cells in a wide variety of species. Functions mediated by calcium channels include contraction of muscle, release of neurotransmitters and hormones by neurons and neuroendocrine cells, and control of gene transcription. They are targets for modulation by many intracellular signaling pathways including G proteins and phosphorylation. Calcium channels play pivotal roles in many human diseases, particularly of the cardiac and nervous systems, including pain, seizure, hypertension and migraine. Pharmacological blockers for some types of calcium channels are known, including clinically used drugs for hypertension and pain. In some cases such calcium channel blockers are highly selective for specific types of calcium channels, but there is great potential for developing more selective and more potent drugs targeting calcium channels.
TargetMol®'s Calcium Antagonist Library collects the reported calcium channel blockers and agonists, and is an ideal tool for screening more selective and potent drugs targeting calcium channels.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	1,650.00
250 µL * 10 mM (in DMSO)	USD	2,775.00
1 mg	USD	2,775.00

Cell Cycle Compound Library

Catalog No. L8100 — 302 compounds

Cell cycle, the ordered sequence of events that occur in a cell in preparation for cell division, is also divided into two periods: interphase and the mitotic (M) phase. Interphase itself is split into different phases: G1 phase, S phase and G2 phase. Cell Cycle related compounds rely on different mechanisms of action to regulate the normal progression of the cell cycle. Some of these compounds interfere with CDK/cyclin complexes leaving cells stuck at the G2/M phase border, while others affect CaMKII phosphorylation, inducing arrest at the G1 phase. Other mechanisms of action include interference with RNA function and inhibition of protein synthesis. Many of these compounds ultimately induce apoptosis as a result of their interruption of the cell cycle. This library can be used for anticancer drug screening.
The TargetMol®'s Cell Cycle Compound Library, a unique collection of 302 cell cycle related compounds, can be used for research in cell cycle and related drug screening.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	4,530.00
250 µL * 10 mM (in DMSO)	USD	7,852.00
1 mg	USD	7,852.00

Chemokine Inhibitor Library

Catalog No. L7600 — 35 compounds

Chemokines are a family of small proteins inducing directed cell migration via specific chemokine receptors, which play important roles in a variety of biological and pathological processes, such as immune surveillance, development, wound healing, bacterial infection, inflammatory reaction, tumor progression and metastasis, etc. Therapeutic strategies based on modulation of chemokine receptor pathways were reported to be promising clinical strategies in the treatment of inflammatory diseases, such as multiple sclerosis and atherosclerosis, psoriasis, inflammatory skin diseases and atopic dermatitis, as well as viral infections, including HIV. Approximately 20 chemokine receptors and 50 chemokines have been identified in humans. Chemokines and their receptors are divided into four families based on the pattern of cysteine residues: CXC, CC, CX3C and XC, where C represents the cysteine and X represents non-cysteine amino acids. Chemokine receptors are seven-transmembrane spanning proteins coupled to G-protein-coupled-receptors (GPCRs). These receptors are named based on the chemokine ligands to which they bind. For example, CXC receptors (CXCR1, 2, 3, 4, 5) bind CXC chemokines, CC receptors (CCR1, 2, 3, 4, 5, 6, 7, 8, 9) bind CC chemokines; CX3C receptor binds CX3C chemokine and lastly, the XC receptor binds the C chemokine. Advances in basic chemokine research have indicated that chemokines and their receptors are the highly promising drug targets for inflammatory and immunological diseases. Antagonizing the chemokine receptor interaction is considered to be beneficial in inflammatory disorders. Currently various chemokine receptor blockers range from monoclonal antibodies, modified chemokines, and low molecular weight receptor antagonists.
TargetMol® collects 35 compounds targeting chemokines or chemokine receptors as Chemokine Inhibitor Library, which can be used for research in immune-mediated diseases, and drug screening.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	2,009.00
250 µL * 10 mM (in DMSO)	USD	2,968.00
1 mg	USD	2,968.00

Cytokine Inhibitor Library

Catalog No. L3600 — 182 compounds

Cytokines are a broad and loose category of small proteins (~5–20 kDa) that are important in cell signaling, modulate the balance between humoral and cell-based immune responses, and are heavily involved in autoimmune and inflammatory diseases. Blocking cytokine signaling pathways by biologics has shown clinical effectiveness in these diseases.
Cytokines act through receptors and activate related signaling to modulate gene expression and cell functions. Cytokine receptors activate many signaling pathways: JAK-STAT, NF-kB, MAPK, PI3K, etc. A number of small molecular weight inhibitors targeting cytokine signaling have been identified as research progresses and some are approved to be marketed. Cytokines Inhibitors Library from TargetMol®, containing 182 compounds targeting cytokine signaling, can be used for high throughput and high content screening for drug discovery.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	4,282.00
250 µL * 10 mM (in DMSO)	USD	6,060.00
1 mg	USD	6,060.00

Cytoskeletal Signaling Pathway Compound Library

Catalog No. T002-00000001 — 343 compounds

The cytoskeleton is a complex, dynamic network of interlinking protein filaments present in the cytoplasm of all cells, including bacteria and archaea. It extends from the cell nucleus to the cell membrane and is composed of similar proteins in various organisms. In eukaryotes, it is composed of three main components, microfilaments, intermediate filaments and microtubules, and these are all capable of rapid growth or disassembly dependent on the cell's requirements. Microfilament functions include cytokinesis, amoeboid movement, cell motility, changes in cell shape, endocytosis and exocytosis, cell contractility, and mechanical stability. Microtubules provide structure and shape to eukaryotic cells and help localize membrane-enclosed organelles. Intermediate filaments have great tensile strength, and their main function is to enable cells to withstand the mechanical stress that occurs when cells are stretched.
The cytoskeleton is responsible for contraction, cell motility, movement of organelles and vesicles through the cytoplasm, cytokinesis, establishment of the intracellular organization of the cytoplasm, establishment of cell polarity, and many other functions that are essential for cellular homeostasis and survival. Many diseases have now been associated with abnormalities in cytoskeletal and nucleoskeletal proteins, including neurodegeneration such as Alzheimer's Disease (AD) with the accumulation of amyloid-beta peptide, and the intracellular neurofibrillary tangles that composed of paired helical filaments of the microtubule-associated protein, tau; cancer (invasion) with cytoskeleton aberration like reduced microtubule polymerization, etc.
TargetMol®'s Cytoskeletal Signaling Pathway Compound Library collects 343 compounds related to cytoskeletal regulation with targets on Microtubule/Tubulin, Kinesin, PKC, MAPK, etc. It can be used for research in cytoskeletal signaling pathway, cytoskeleton-associated disease, and drug discovery.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	5,710.00
250 µL * 10 mM (in DMSO)	USD	9,378.00
1 mg	USD	9,378.00

Endoplasmic Reticulum Stress Compound Library

Catalog No. L9700 — 155 compounds

The endoplasmic reticulum (ER) is the cellular organelle that is critical for protein folding and secretion, calcium homeostasis, and lipid biosynthesis. The ER is the site of multiple post-translational modifications such as glycosylation and disulfide bond formation. It is also the organelle in which proteins are folded into their proper conformation and in which multi-subunit proteins are assembled. Endoplasmic reticulum stress (ER stress), such as unfolded protein response (UPR) and ER overload response (EOR), occurs when proteins are not properly folded or conformed (misfolded protein) or homeostasis cannot be maintained such as disturbances in redox regulation, calcium regulation, glucose deprivation, and viral infection. As a result, ER-localized chaperones such as glucose-regulated proteins (GRP78, GRP94, etc.) are induced, protein synthesis is slowed down, and a protein degrading system is initiated. However, excessive and prolonged stresses lead cells to caspase-12 mediated apoptosis.
ER stress occurs not only in both normal and pathophysiological conditions, but has also been implicated in multiple disorders such as cancers, type 2 diabetes, ischemia, viral infection, and neurodegenerative disorders. ER stress can also be induced by hypoxia. This has implications for solid tumors which usually exhibit hypoxia in their cores. Insulin resistance is also associated with ER stress and the treatment of type 2 diabetic mice with chemical chaperones which assist protein folding in the ER restored insulin sensitivity. It has also been proposed that agents that cause ER stress can be used directly as chemotherapeutic agents.
TargetMol®'s Endoplasmic Reticulum Stress Compound Library collects 155 ER stress 0 related compounds, targeting different targets in ER stress signaling pathway such as PERK, IRE1, ATF6, GRP78, etc. It is an effective tool for research in endoplasmic reticulum stress and related diseases.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	2,480.00
250 µL * 10 mM (in DMSO)	USD	4,495.00
1 mg	USD	4,495.00

Epigenetics Compound Library

Catalog No. L1200 — 1016 compounds

Product Description

Epigenetics is the study of molecular processes that influence the flow of information between a constant DNA sequence and variable gene expression patterns. This includes investigation of nuclear organization, DNA methylation, histone modification and RNA transcription. Epigenetic processes can result in intergenerational (heritable) effects and clonal propagation of cell identity without any mutational change in DNA sequence. Epigenetics has the potential to be a key element in a paradigm change of our understanding of aging, development, cancer, heart disease, psychological disorders, and other diseases. For example, Epigenetic modifications have a considerable effect on cancer. Changes in the pattern of histone modifications in the promoter sequences as epigenetic regulation lead to changes in chromatin structure thus may be the cause of altered gene expression by activation of oncogenes.
The Epigenetics Compound Library by TargetMol®, containing 1016 compounds related to epigenetic regulation, can be used for research in epigenetics, high throughput screening and high content screening for new drugs in epigenetic modification.

Product Advantage

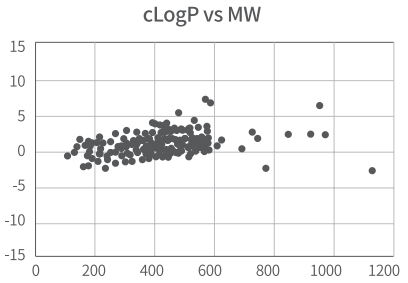
- A unique collection of 1016 compounds related to epigenetic regulation for high throughput screening(HTS)and high content screening(HCS) for new drugs;
- Targets include HDAC, SIRT, HAT, and HMT, etc.;
- Some of the compounds are approved by FDA;
- Detailed compound information with structure, target, activity, IC50 value, and brief introduction;
- NMR and HPLC/LCMS were validated to ensure high purity and quality and reduce false-positive rate.

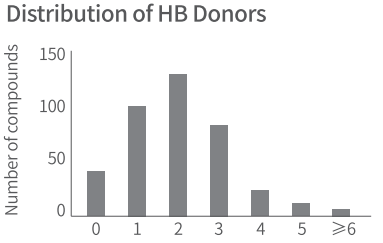
Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	15,120.00
250 µL * 10 mM (in DMSO)	USD	25,168.00
1 mg	USD	25,168.00

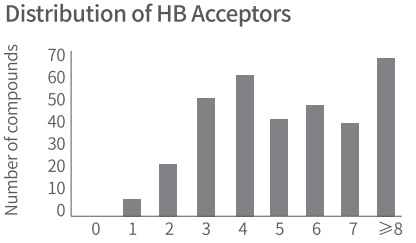
Drug-Like Properties

% of compounds compliant with Lipinski' s Rules

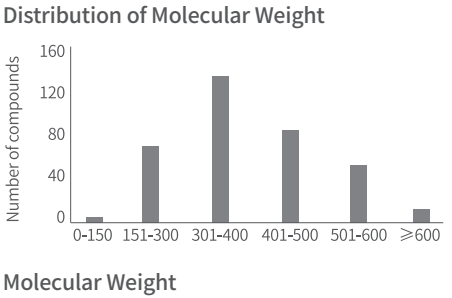
PhysChem Properties	% Compounds
<5 H-Bond donors	95
<10 H-Bond acceptors	94
cLogP<5	92
MW<500	82

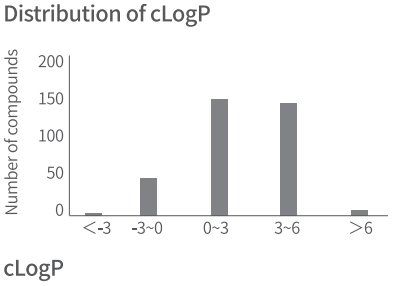




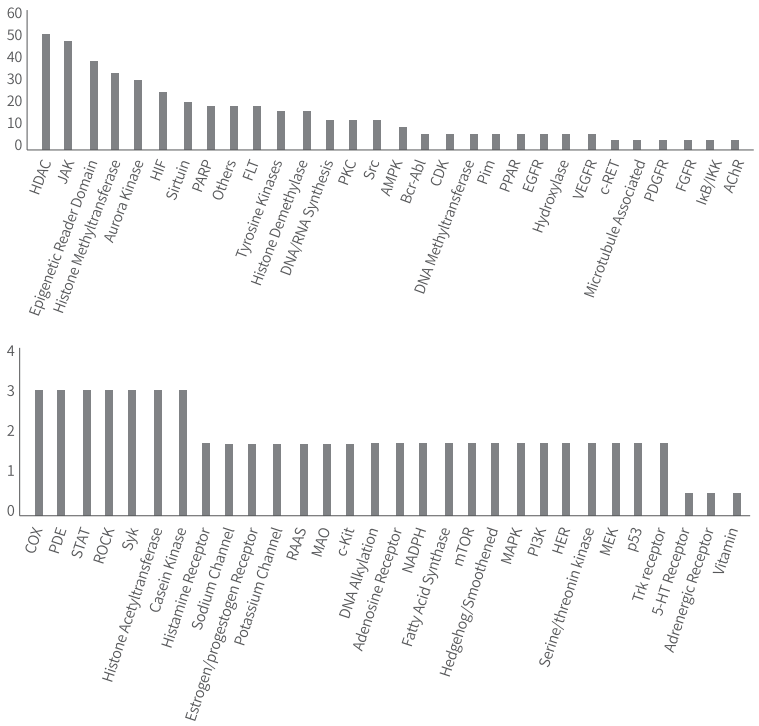


Drug-Like Properties

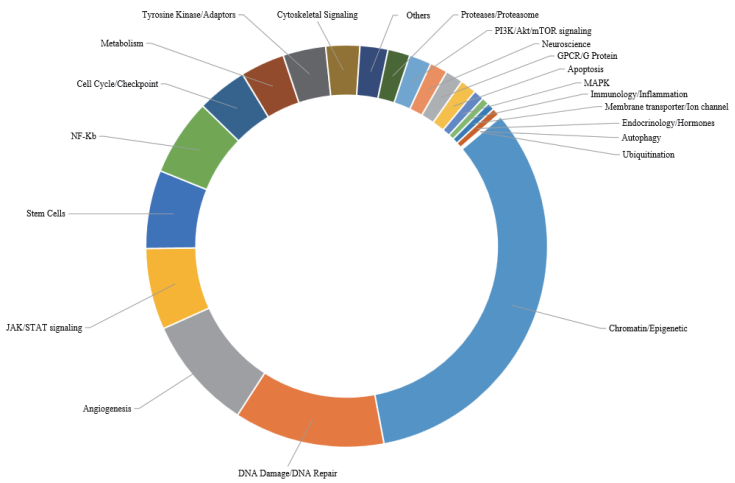




Target Composition



Signaling Pathways



Exosome Compound Library

Catalog No. L9420 — 45 compounds

Extracellular vesicles are important mediators of protein, mRNA, miRNA, and lipid transport to complete intercellular communication pathways and are classified into three categories based on their size and biogenesis, including exosomes, microvesicles, and apoptotic vesicles. Among them, exosomes are packed vesicles of approximately 40-100 nm in diameter, secreted by a variety of cells containing specific proteins, lipids, cytokines, or genetic material, which are widely found in various body fluids, including blood, saliva, urine, cerebrospinal fluid, semen, breast milk, amniotic fluid, ascites, vaginal/alveolar lavage fluid, etc.
Exosomes are involved in many biological functions, including immune regulation, where B-lymphocytes secrete exosomes with antigen-presenting proteins to induce immune responses in T-lymphocytes. It contributes to the formation as well as the development of some diseases, such as neurodegenerative Alzheimer's disease, and facilitates viral infection and transmission, such as HIV, which utilizes exosomes to find the most suitable cells for infection and transmission. Exosomes are directly involved in the development and progression of cancer. By carrying oncogenic factors like proto-oncoproteins and RNAs that cause cancer in recipient cells, exosomes can induce metastasis and spread of cancer cells. At the same time, it can inhibit the activity of immune cells (cause immune apoptosis) so that cancer cells can escape from the immune system.
In conclusion, research on exosomes can provide new ideas and therapies for the treatment of certain diseases. TargetMol has collected 45 exosome-related compounds for customers engaged in exosome research to help you with your research.

Pack Size		Price
100 μL * 10 mM (in DMSO)	USD	964.00
250 μL * 10 mM (in DMSO)	USD	1,446.00
1 mg	USD	1,446.00

Ferroptosis Compound Library

Catalog No. L8700 — 694 compounds

Ferroptosis is a type of programmed cell death dependent on iron and characterized by the accumulation of lipid peroxides, and is genetically, biochemically and morphologically distinct from other forms of regulated cell death such as apoptosis, necroptosis, and autophagic cell death. It is characterized morphologically by the presence of smaller than normal mitochondria with condensed mitochondrial membrane densities, reduction or vanishing of mitochondria crista, and outer mitochondrial membrane rupture. Misregulated ferroptosis has been implicated in multiple physiological and pathological processes, including cancer cell death, neurotoxicity, neurodegenerative diseases, acute renal failure, drug-induced hepatotoxicity, hepatic and heart ischemia/reperfusion injury, and T-cell immunity. Understanding the molecular mechanisms and signaling pathways of ferroptosis may provide new diagnostic and therapeutic approaches to regulate cell survival and death in human disease.
TargetMol® collects 694 compounds related to ferroptosis signaling pathway with targets including GPX4, System Xc $^-$, HSPB1, NRF2, VDAC2/3, Ras, TFR1, NOX, p53, CARS, ROS, SLC7A11, etc. Iron chelators and lipid peroxidation inhibitors are also included in this library.

Pack Size		Price
100 μL * 10 mM (in DMSO)	USD	11,555.00
250 μL * 10 mM (in DMSO)	USD	18,976.00
1 mg	USD	18,976.00

GPCR Compound Library

Catalog No. L1500 — 1473 compounds

G-protein-coupled receptors (GPCRs) are the largest and most diverse group of membrane receptors in eukaryotes that detect molecules outside the cell and activate internal signal transduction pathways and, ultimately, cellular responses. GPCRs are involved in nearly every aspect of animal life, from early development and heart function to neuronal activity. Mutations in GPCRs are linked to a number of human diseases. GPCRs are an important drug target and approximately 34% of the marketed drugs target 108 members of this family, with an additional 66 receptors targeted by agents that are/were in clinical trials. GPCR-based drug discovery remains active campaign in major pharmaceutical companies. To date, more than 140 orphan GPCRs, whose endogenous ligands are unknown, are the focus of an intense drug discovery effort in many programs.
Specifically, the optimal ligands to GPCRs need to possess high affinity and specificity for the target protein, and reasonable membrane permeability for biological activity in whole-cell assays and in vivo models. GPCR Compound Library from TargetMol®, is a focused small molecule library developed against particular GPCRs containing 1473 GPCR-active agents for GPCR drug discovery.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	16,707.00
250 µL * 10 mM (in DMSO)	USD	23,790.00
1 mg	USD	23,790.00

GPCR Compound Library Plus

Catalog No. L1580 — 403 compounds

G-protein-coupled receptors (GPCRs) are the largest and most diverse group of membrane receptors in eukaryotes that detect molecules outside the cell and activate internal signal transduction pathways and, ultimately, cellular responses. GPCRs are involved in nearly every aspect of animal life, from early development and heart function to neuronal activity. Mutations in GPCRs are linked to a number of human diseases. GPCRs are an important drug target and approximately 34% of the marketed drugs target 108 members of this family, with an additional 66 receptors targeted by agents that are/were in clinical trials. GPCR-based drug discovery remains active campaign in major pharmaceutical companies. To date, more than 140 orphan GPCRs, whose endogenous ligands are unknown, are the focus of an intense drug discovery effort in many programs.
GPCR Compound Library Plus from TargetMol®, a focused small molecule library, was developed against particular GPCRs containing 403 GPCR-active agents with IC50 less than 3.5 µM for GPCR drug discovery, target identification, and research in signaling pathway.

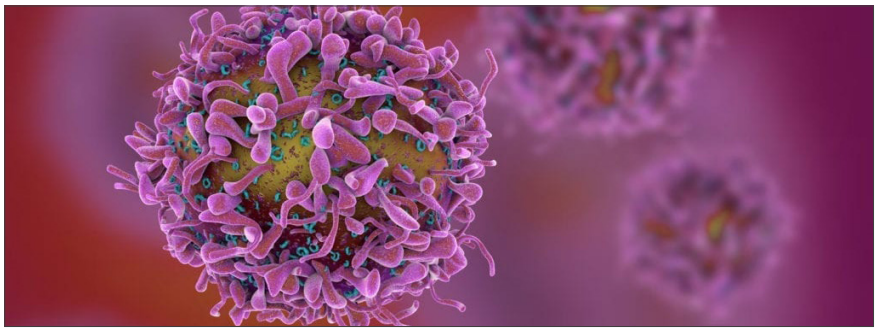
Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	6,008.00
250 µL * 10 mM (in DMSO)	USD	10,214.00
1 mg	USD	10,214.00

HIF-1 Signaling Pathway Compound Library

Catalog No. L8500 — 1071 compounds

Cell signaling is part of any communication process that the governs the basic activities of cells and coordinates all cell actions. The ability of cells to perceive and correctly respond to their microenvironment is the basis of development, tissue repair, and immunity, as well as normal tissue homeostasis. Errors in signaling interactions and cellular information processing are responsible for diseases such as cancer, autoimmunity, and diabetes. By understanding cell signaling, diseases may be treated more effectively.
As a key regulator of the hypoxia response, hypoxia-inducible factor-1 (HIF-1) has been attracting more attention from scientists. HIF-1 is an evolutionarily conserved transcription factor that functions as a main regulator of gene expression in response to hypoxia. HIF-1 is functionally heterodimeric, composed of HIF-1β and one of three α subunits (HIF-1α, HIF-2α, or HIF-3α). All subunits are part of the basic helix-loop-helix superfamily of transcription factors, but their activity is primarily controlled by cellular levels of the HIF-1α subunit. As a transcriptional factor, the heterodimer HIF-1 recognizes and binds to the consensus sequence 5’-(A/G) CGTG-3’ named hypoxia-responsive elements (HREs) to activate the transcriptional activity of target genes. To date, more than 100 direct target genes of HIF-1 have been uncovered, which have been shown to be functionally involved in tumor metastasis, angiogenesis, energy metabolism, cell differentiation and apoptosis.
Intensive studies have clearly established the hypoxia/HIF signaling pathway as a master regulator of the vascular system. Accordingly, it represents an important therapeutic target for vascular diseases and cancer. Pharmacologically increased HIF function may aid in the treatment of a wide range of diseases, as HIF has been shown to be essential for phenomena as diverse as immune function, cartilage formation, and wound healing. Conversely, inhibition of HIF function could also have many applications: increased levels of HIF are seen in many cancers as well as in some cardiovascular diseases, including stroke, heart attack, and pulmonary hypertension.
To meet the need of research in oxygen-sensing pathways, TargetMol® collects 1071 HIF-1 related small chemicals，involving PI3K-AKT, MAPK, Ubiquitination signaling pathways and targets such as HIF, HIF Prolyl-Hydroxylase, E1/E2/E3 Enzyme, PI3K, MAPK, Proteasome, etc.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	19,278.00
250 µL * 10 mM (in DMSO)	USD	31,855.00
1 mg	USD	31,855.00



Histamine & Melatonin Receptor-Targeted Compound Library

Catalog No. L3300 — 120 compounds

Histamine, an important bioactive molecule, is derived from the decarboxylation of the amino acid histidine. Most histamine in the body is generated in granules in mast cells and in skin, lung and gastrointestinal tract, playing a pivotal role in allergic and inflammatory reactions. Histamine acts as a neurotransmitter within the central nervous system. The histaminergic neurons that secrete histamine are localized in small regions of the hypothalamus, but those neurons send axons widely throughout the brain. Histamine appears to modulate a number of important processes in the brain, including wakefulness, cognitive ability and food consumption. Currently four histamine receptors (H1R-H4R) have been cloned and identified, all of which are G protein-coupled receptors. These different receptors are expressed on different cell types and work through different intracellular signaling mechanisms. Post mortem studies have revealed alterations in histaminergic system in neurological and psychiatric diseases.
Melatonin is a hormone, produced by the pineal gland, a tiny endocrine gland situated at the center of the brain. Melatonin presents several ways of action in the regulation of seasonal reproduction, body weight and energy balance, antiaging, and promoting sleep.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	2,142.00
250 µL * 10 mM (in DMSO)	USD	3,564.00
1 mg	USD	3,564.00

Inhibitor Library

Catalog No. L2000 — 4784 compounds

Cell signaling is part of any communication process that governs the basic activities of cells and coordinates all cell actions. The ability of cells to perceive and correctly respond to their microenvironment is the basis of development, tissue repair, and immunity, as well as normal tissue homeostasis. Errors in signaling interactions and cellular information processing are responsible for diseases such as cancer, auto-immunity, and diabetes. By understanding cell signaling, diseases may be treated more effectively.
Inhibitor library is a unique collection of 4784 compounds, each of which has clear inhibitory targets. It is an effective tool for research in cell signaling pathways and related diseases, and high throughput screening and high content screening for new drugs.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	41,346.00
250 µL * 10 mM (in DMSO)	USD	68,965.00
1 mg	USD	68,965.00

Ion Channel Inhibitor Library

Catalog No. L2300 — 705 compounds

Given the central functional role that the ion channel superfamily plays in human physiology, its membrane localization, and the diverse tissue distribution of different members of the family, it represents an attractive potential target class for drug discovery. Ion channels play a fundamental role in the way cells communicate. This communication between cells allows for the orchestration of physical and mental activities in humans. A number of diseases occur when ion channels do not function properly. Some examples are diabetes, neuropathic pain, cardiovascular diseases, asthma, epilepsy, and neurodegenerative disease, etc.
The Ion Channel Inhibitor Library by TargetMol®, containing 705 compounds targeting ion channels, can be used for research in ion channel, high throughput screening and high content screening for ion channel drug discovery.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	6,333.00
250 µL * 10 mM (in DMSO)	USD	11,175.00
1 mg	USD	11,175.00

JAK-STAT Compound Library

Catalog No. L3700 — 218 compounds

Cell signal transduction is the transmission of molecular signals via various proteins in a signaling cascade, which carries and amplifies the signal. The JAK-STAT signaling pathway communicates information from chemical signals outside of a cell to the cell nucleus, resulting in the activation of genes through a process called transcription. There are three critical parts of JAK-STAT signaling: Janus kinases (JAKs), Signal Transducer and Activator of Transcription proteins (STATs), and receptors (which bind the chemical signals). JAK-STAT signaling pathway is a chain of interactions between proteins in a cell, and is involved in processes such as immunity, cell division, cell death and tumor formation. Disrupted JAK-STAT signaling may lead to a variety of diseases, such as skin conditions, cancers, and disorders affecting the immune system. There are 4 JAK proteins: JAK1, JAK2, JAK3 and TYK2, and there are 7 STAT proteins: STAT1, STAT2, STAT3, STAT4, STAT5A, STAT5B and STAT6.
JAK-STAT Compound Library from TargetMol®, a unique collection of 218 compounds targeting JAK/STAT signaling, can be used for research in JAK/STAT signaling and related drug screening (high throughput and high content screening).

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	3,488.00
250 µL * 10 mM (in DMSO)	USD	6,322.00
1 mg	USD	6,322.00

Tyrosine Kinase Inhibitor Library

Catalog No. L1600 — 2203 compounds

Product Description

In biochemistry, a kinase is an enzyme that catalyzes the transfer of phosphate groups from high-energy, phosphate-donating molecules (ATP) to specific substrates. This process is known as phosphorylation. The protein kinases make up the majority of all kinases and are widely studied. A protein kinase modifies other molecules, mostly proteins, by phosphorylation to regulate the majority of cellular pathways, especially those involved in signal transduction. Various other kinases act on small molecules such as lipids, carbohydrates, amino acids, and nucleotides, either for signaling or to prime them for metabolic pathways.
TargetMol®'s Tyrosine Kinase Inhibitor Library, containing 2203 kinase inhibitors, can be used for research in chemical genomics, pharmacological study, and drug screening for related diseases.

Product Advantage

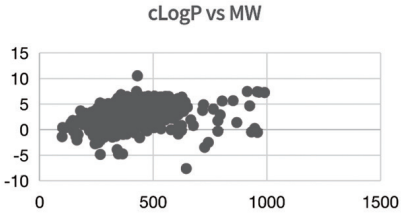
- A unique collection of 2203 kinase inhibitors for high throughput and high content screening for drug discovery;
- Targets include MAPK, PI3K, JAK, STAT, CDK, MEK, Insulin/IGF receptors, CaM Kinase ll, PKA, JNK, PKC, RAF, EGFR, SAPK, GSK, MLCK Src-family, IKK, PDGFR, VEGFR, etc;
- Bioactivity and safety confirmed by preclinical research and clinical trials, and some of them are approved by FDA;
- Detailed compound information with structure, target, activity, IC50 value, and brief introduction;
- NMR and HPLC/LCMS validated to ensure high purity and quality and reduce false-positive rate.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	28,522.00
250 µL * 10 mM (in DMSO)	USD	46,734.00
1 mg	USD	46,734.00

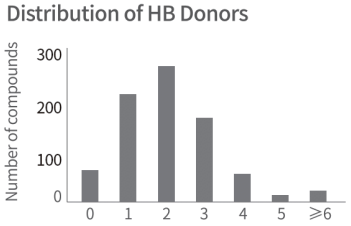
Drug-Like Properties

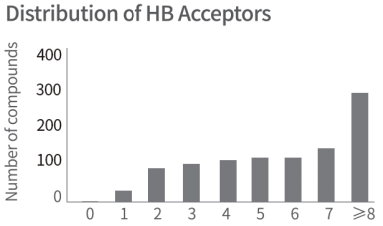
% of compounds compliant with Lipinski' s Rules

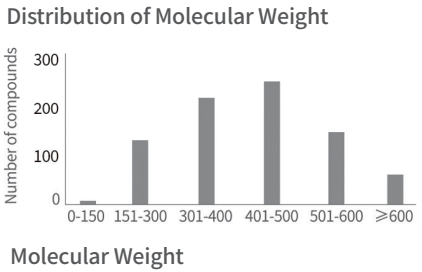
PhysChem Properties	% Compounds
<5 H-Bond donors	95
<10 H-Bond acceptors	88
cLogP<5	89
MW<500	77

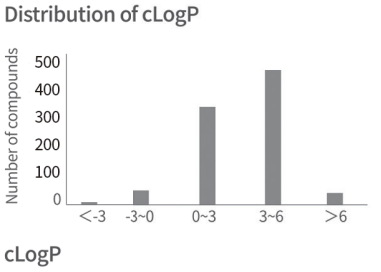


Drug-Like Properties

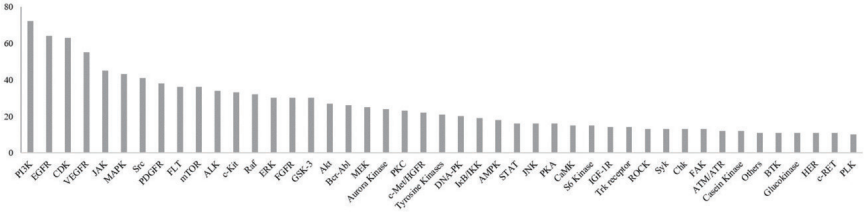




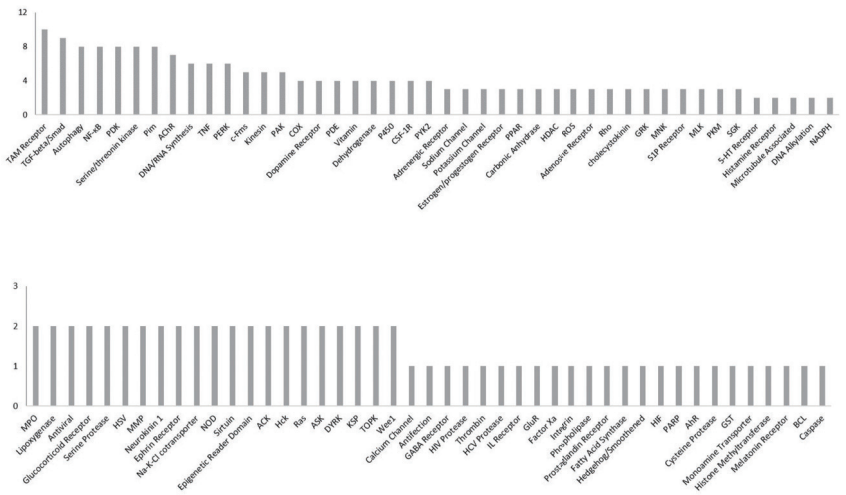




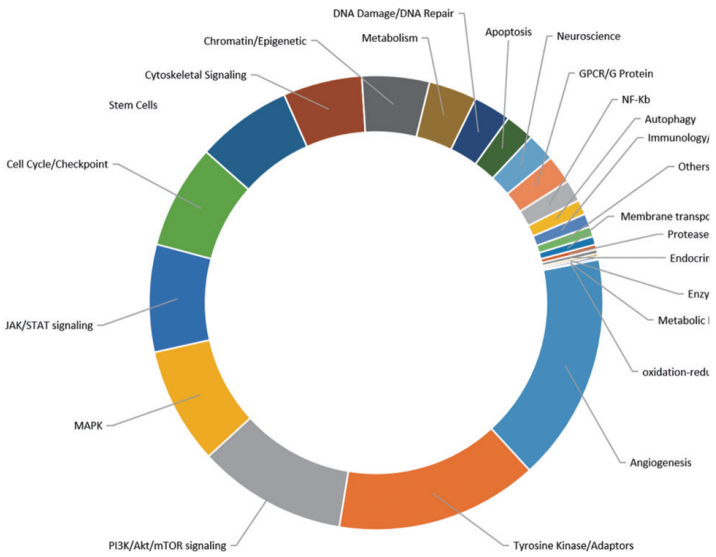
Target Composition



Target Composition

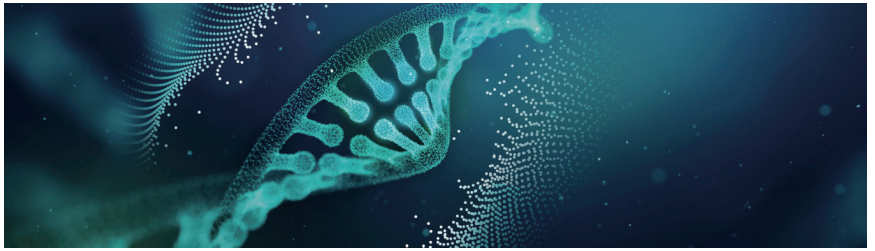


Signaling Pathways



Other related Compound Libraries

Compound Library	Size	Comments
Tyrosine Kinase Inhibitor Library L2200	640	A unique collection of 640 tyrosine kinase inhibitors targeting tyrosine kinase signaling; Targets include c-Kit, c-Met, EGFR, FGFR, SRC, JAK, SYK, Btk, Bcr-Abl, etc.
MAPK Inhibitor Library L1400	234	A unique collection of 234 compounds targeting MAPK signaling;Effective tool for studying cell growth, proliferation, and apoptosis; Targets include ERK, JNK, MEK, p38, MAPK, Raf, RSK, MNK, etc.
PI3K/Akt/mTOR Compound Library L1300	319	A unique collection of 319 compounds targeting PI3K/Akt/mTOR signaling for research in PI3K/Akt/mTOR signaling; Effective tool for studying cell growth, proliferation, and apoptosis; Targets include AKT, AMPK, mTOR, PI3K, ATR/ATM, etc.
JAK-STAT Compound Library L3700	218	A unique collection of 218 JAK/STAT signaling targeted compounds for high throughput and high content screening; Effective tool for studying the JAK/STAT targets and target identification.
TGF-beta/Smad Compound Library L4100	116	A unique collection of 116 TGF-beta/Smad signaling targeted compounds; Effective tool for research in TGF-beta/Smad signaling, related drug screening, and target identification.
Wnt/Hedgehog/Notch Compound Library L4300	136	A unique collection of 136 Wnt/Hedgehog/Notch signaling targeted compounds; Effective tool for research in Wnt/Hedgehog/Notch signaling and target identification.



MAPK Inhibitor Library

Catalog No. L1400 — 234 compounds

Mitogen-activated protein kinases (MAPKs) are a highly conserved family of serine/threonine protein kinases involved in a variety of fundamental cellular processes such as proliferation, differentiation, motility, stress response, apoptosis, and survival. A broad range of extracellular stimuli including mitogens, cytokines, growth factors, and environmental stressors stimulate the activation of one or more MAPKK kinases (MAPKKKs) via receptor-dependent and -independent mechanisms. MAPKKKs then phosphorylate and activate a downstream MAPK kinase (MAPKK), which in turn phosphorylates and activates MAPKs.
The MAPK Inhibitor Library by TargetMol®, containing 234 compounds targeting MAPK signaling, can be used for research in MAPK signaling, and drug screening for related diseases.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	3,920.00
250 µL * 10 mM (in DMSO)	USD	6,670.00
1 mg	USD	6,670.00

Methylation Compound Library

Catalog No. L3510 — 125 compounds

Methylation is an important way of protein and nucleic acid modification that regulates gene expression and is closely related to many diseases such as cancer, aging, and Alzheimer's disease. It is an important field of study in epigenetics. The most common methylation modifications are DNA methylation and histone methylation
DNA methylation, the addition of methyl groups to DNA, was one of the first methylation modifications discovered. The modification occurs specifically at the CpG site, where cytosine is attached to guanylate via phosphate. Numerous studies have shown that DNA methylation can cause changes in chromatin structure, DNA conformation, DNA stability and the way DNA interacts with proteins, thereby controlling gene expression.
Histone methylation refers to the methylation that occurs at the N-terminal arginine Arg(R) or lysine Lys(K) residues of H3 and H4 histones and is mediated and catalyzed by histone methyltransferases. Histone methylation mainly causes heterochromatin formation, gene imprinting, X chromosome inactivation and transcriptional regulation.
TargetMol® Methylation Compound Library is a collection of 125 methylation-related compounds that can be used for research in epigenetics, differentiation, aging, cancer, and more.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	2,014.00
250 µL * 10 mM (in DMSO)	USD	3,367.00
1 mg	USD	3,367.00

Microtubule-Targeted Compound Library

Catalog No. L1110 — 58 compounds

Microtubules (MTs) are cylindrical polymers of α- and β-tubulin heterodimers. These polymers are highly dynamic and their polymerization dynamics are tightly regulated through the binding of microtubule-associated proteins (MAPs). Microtubule polymerization and depolymerization dynamics drive chromosome congression and spindle formation during cell division, which are used to pull eukaryotic chromosomes apart. Microtubules are very important in a number of cellular processes, such as maintaining the structure of the cell, cell division, signaling transduction, transportation, etc.
Microtubules have long been considered an ideal target for anticancer drugs because of the essential role they play in mitosis, forming the dynamic spindle apparatus. Microtubule-targeting anticancer drugs are among the most effective anticancer therapeutics used in the clinic today. Microtubule-targeting agents act primarily by altering MT dynamics. This interference with microtubule dynamics can have the effect of stopping a cell's cell cycle and can lead to programmed cell death or apoptosis. They are roughly classified into microtubule-stabilizing agents, such as taxanes (paclitaxel) or epothilones. They block dynamic instability by stabilizing GDP-bound tubulin in the microtubule to inhibit the mitosis and induce apoptosis; microtubule-destabilizing agents, such as vinca alkaloids, Nocodazole, combretastatin, and colchicine.
TargetMol®'s Microtubule-targeted Compound Library collects 58 compounds targeting microtubules that can be used in microtubule-related mechanism study and drug development.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	1,190.00
250 µL * 10 mM (in DMSO)	USD	1,785.00
1 mg	USD	1,785.00

Mitochondria-Targeted Compound Library

Catalog No. L5300 — 168 compounds

The mitochondrion is a double-membrane-bound discrete organelle found in most eukaryotic organisms, generating most of the cell's supply of adenosine triphosphate (ATP) and controlling the cellular basal metabolic rate, it is also called the cell's powerhouses. In addition to supplying cellular energy, mitochondria are the major source of ROS (reactive oxygen species) that reflect the level of cellular oxidative stress and play an important role in mitochondria ROS signaling such as apoptosis, proliferation, and aging, etc. In addition, the fine modulation of mitochondrial calcium (Ca2+) homeostasis plays a fundamental role in many of the processes involving this organelle. Mitochondrial Ca2+ accumulation is a tightly controlled process that regulates functions as diverse as aerobic metabolism and induction of cell death. Mitochondrial DNA mutations may lead to many mitochondrial metabolic disorders, and are thought to contribute to aging by promoting apoptosis. Mitochondria therefore represent an attractive drug target for metabolic diseases, neurodegeneration, or hyperproliferative diseases (cancer). A number of preclinical and clinical data have shown that mitochondria as drug targets have great potential. Small molecule drugs or biologics can act on mitochondria through various pathways including ETC inhibition, OXPHOS uncoupling, mitochondrial Ca2+ modulation, and oxidative stress control via decreased or increased mitochondrial ROS accumulation.
Mitochondria-Targeted Compound Library from TargetMol®, a unique collection of 168 compounds targeting mitochondria, can be used for research in mitochondrial medicine and related target study.

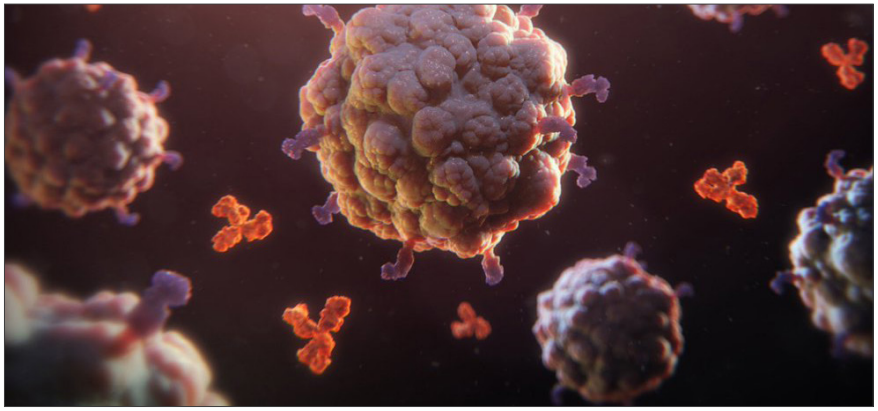
Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	3,652.00
250 µL * 10 mM (in DMSO)	USD	6,208.00
1 mg	USD	6,208.00

Neuronal Signaling Compound Library

Catalog No. L2600 — 1740 compounds

Communication between and within neurons is critical for all functions of the nervous system, from development to aging, through health and disease. The last decade has seen huge advances in our knowledge of the molecular, cellular and systematic signaling pathways within the nervous system. There have been significant breakthroughs in studies on the signaling pathways that underlie neurogenesis, addiction and autism spectrum disorders, and the pathophysiology and treatment of mood disorders. G protein-coupled receptors(GPCRs), including 5-HT receptors, histamine receptors, opioid receptors, are the largest family of signaling proteins to neuronal signaling. Changes in the GPCRs functioning can cause many Neurological Disorders; Notch signaling is essential for proliferation, survival, self-renew, and differentiation of neural stem cells (NSCs). Notch signaling in neurons, glia and NSCs may be involved in pathological changes that occur in disorders such as stroke, Alzheimer's disease and CNS tumors. Therefore, the potential of agents that target notch signaling could be used as therapeutic interventions for several different CNS disorders.
The Neuronal Signaling Compound Library by TargetMol®, containing 1740 compounds targeting CNS signaling, can be used for high throughput screening and high content screening for new drugs in neurological disorders.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	16,823.00
250 µL * 10 mM (in DMSO)	USD	27,847.00
1 mg	USD	27,847.00

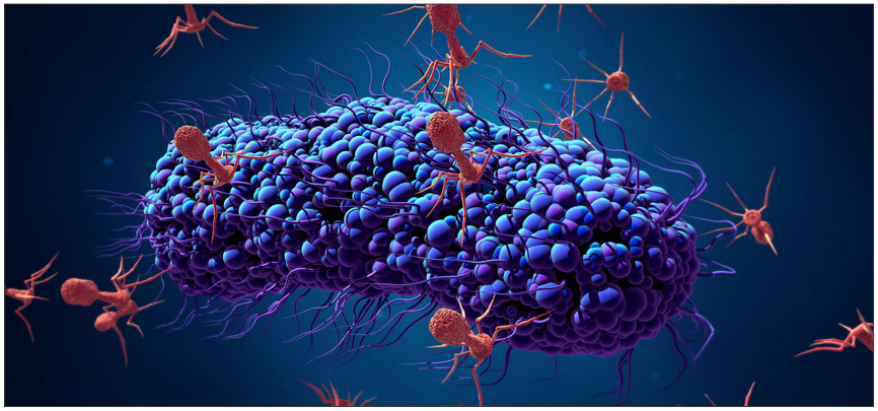


Neurotransmitter Receptor Compound Library

Catalog No. L2610 — 956 compounds

A neurotransmitter receptor (also known as a neuroreceptor) is a membrane receptor protein that is activated by a neurotransmitter. Chemicals on the outside of the cell, such as a neurotransmitter, can bump into its corresponding receptor in the membrane, bind and trigger other events inside the cell. A neurotransmitter receptor is a class of receptors that specifically binds with neurotransmitters as opposed to other molecules. Neurotransmitter (NT) receptors are located on the surface of neuronal and glial cells.
There are two major types of neurotransmitter receptors: ionotropic and metabotropic. Ionotropic means that ions can pass through the receptor, whereas metabotropic means that a second messenger inside the cell relays the message (i.e. metabotropic receptors do not have channels). Metabotropic receptors are in fact G protein-coupled receptors. Ionotropic receptors are also called Ligand-gated ion channels and they can be excited by neurotransmitters like glutamate and aspartate. There are several major classes of neurotransmitters: Adrenergic, Dopaminergic, GABAergic, Glutaminergic, Histaminergic, Cholinergic, Opioid, Serotonergic, and Glycinergic.
In the brain, most drug targets consist of signaling proteins that go awry in central nervous system diseases, for example with autism in childhood, schizophrenia in adolescence, or Alzheimer's disease in old age. The aim of drug treatment is to correct the inappropriate behavior of these proteins and restore normal brain function. Understanding the effects of neurotransmitters is extremely important in therapeutics. All psychiatric drugs act by affecting neurotransmitters. Understanding their mechanism of action and adverse effects is key to developing new drugs for neurological diseases.
The TargetMol® neurotransmitter receptor compound library contains 956 CNS receptor ligands, which is ideal for screening or identifying recombinant orphan G protein-coupled receptors, target validation, secondary screening, validating new assays, and for routine pharmacological applications.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	15,774.00
250 µL * 10 mM (in DMSO)	USD	23,680.00
1 mg	USD	23,680.00



NF-κB Signaling Compound Library

Catalog No. L3800 — 452 compounds

Nuclear factor-κB (NF-κB), a collective term for a family of transcription factors, includes five subunits: NF-κB1 (p50/p105), NF-κB2 (p52/p100), p65 (RelA), RelB, and c-Rel. The homodimers or heterodimers formed by two subunits bind to specific sequences known as the κB site on their target genes for DNA interaction and transcriptional activation. How NF-κB selectively recognizes a small subset of relevant κB sites from the large excess of potential binding sites is a critical step for stimulus-specific gene transcription (The fine-tuning of the NF-B DNA binding activity). While in an inactivated state, NF-κB is located in the cytosol complexed with the inhibitory protein IκBα. Through the intermediacy of integral membrane receptors, a variety of extracellular signals can activate the enzyme IκB kinase(IKK). IKK, in turn, phosphorylates the IκBα protein, which results in ubiquitination, dissociation of IκBα from NF-κB, and eventual degradation of IκBα by the proteasome. The activated NF-κB is then translocated into the nucleus where it binds to specific sequences of DNA called response elements (RE). The DNA/NF-κB complex then recruits other proteins such as coactivators and RNA polymerase, which transcribe downstream DNA into mRNA. A large array of genes involved in different processes of the immune and inflammatory responses, such as TNF-α, IL-1β, IL-6, and IL-8, chemokines, adhesion molecules, clone stimulating factors, is mediated by NF-κB. In TNF-α–induced apoptosis, TRAF1, TRAF2, XIAP, c-IAP1, and c-IAP2 were identified as gene targets of NF-kB transcriptional activity.
NF-κB Signaling Compound Library from TargetMol®, a unique collection of 452 small molecules targeting NF-κB signaling, can be used for research in NF-κB signaling and high throughput screening and high content screening.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	8,136.00
250 µL * 10 mM (in DMSO)	USD	14,464.00
1 mg	USD	14,464.00

Nuclear Receptor Inhibitor Library

Catalog No. L1510 — 298 compounds

Nuclear receptors are a class of proteins, different from membrane receptors located in the cell membrane, found within cells that are responsible for sensing steroid and thyroid hormones and certain other molecules. Nuclear receptors have the ability to directly bind to DNA and regulate the expression of adjacent genes, hence these receptors are classified as transcription factors, thereby controlling the development, homeostasis, and metabolism of the organism. Over the last 15 years a growing number of nuclear receptors have been identified that coordinate genetic networks regulating lipid metabolism and energy utilization and underlie the pathogenesis of metabolic diseases, such as obesity, type II diabetes, hypertension, and cardiovascular disease.
TargetMol® collects 298 reported compounds targeting nuclear receptors as Nuclear Receptor Inhibitor Library, which can be used for research in nuclear receptor signaling and related diseases, and high throughput and high content screening for drug discovery.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	3,615.00
250 µL * 10 mM (in DMSO)	USD	6,358.00
1 mg	USD	6,358.00

Phosphatase Inhibitor Library

Catalog No. L9100 — 39 compounds

The phosphatase inhibitor compound library is a collection of 39 phosphatase inhibitors with known activity, which can be used for drug screening, chemical genomics, pharmacological analysis, etc.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	1,829.00
250 µL * 10 mM (in DMSO)	USD	2,707.00
1 mg	USD	2,707.00

PI3K-AKT-mTOR Compound Library

Catalog No. L1300 — 319 compounds

The PI3K/AKT/mTOR pathway is an intracellular signaling pathway important in regulating the cell cycle. Therefore, it is directly related to cellular quiescence, proliferation, cancer, and longevity. Phosphatidylinositol 3-kinase (PI3K), AKT, a serine/threonine protein kinase also known as protein kinase B (PKB), and mammalian target of rapamycin (mTOR) are 3 major nodes in the pathway. PI3K activation phosphorylates and activates AKT, localizing it in the plasma membrane. AKT can have a number of downstream effects such as activating CREB, inhibiting p27, localizing FOXO in the cytoplasm, activating PtdIns-3ps, and activating mTOR which can affect transcription of p70 or 4EBP1. mTOR is a component of the PI3K/AKT cell survival pathway that monitors the availability of nutrients, mitogenic signals and cellular energy and oxygen levels. A major regulator of the autophagic process, and alterations in components of the mTOR pathway have a major role in tumor progression. Therefore, mTOR is an appealing therapeutic target in many tumors. Encouraging data from preclinical studies have offered new opportunities to fully exploit the therapeutic potential of mTOR targeting in cancer treatments.
The PI3K/Akt/mTOR Compound Library by TargetMol®, containing 319 compounds targeting PI3K/Akt/mTOR signaling, can be used for high throughput screening and high content screening for new drugs.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	9,129.00
250 µL * 10 mM (in DMSO)	USD	14,390.00
1 mg	USD	14,390.00

Potassium Channel Blocker Library

Catalog No. L7300 — 90 compounds

Potassium channels are the most widely distributed type of ion channel and are found in virtually all living organisms. They form potassium-selective pores that span cell membranes. Furthermore, potassium channels are found in most cell types and control a wide variety of cell functions, such as regulation of cellular excitability, neurotransmitter release, protecting cardiac myocytes, and antiarrhythmic function, and are involved in learning and memory process, and temperature control. Potassium channel blockers are a class of drugs that act by inhibition of potassium efflux through cell membranes, including inorganic ions (Cs, Ba) and organic molecules (TEA, 4-AP), toxins (scorpion venoms, snake venoms, and bee venoms), and potassium channel blockers in clinical use.

Pack Size		Price
100 μL * 10 mM (in DMSO)	USD	1,959.00
250 μL * 10 mM (in DMSO)	USD	3,324.00
1 mg	USD	3,324.00

Protease Inhibitor Library

Catalog No. L1100 — 295 compounds

Protease inhibitors are molecules that inhibit the function of proteases (enzymes that aid the breakdown of proteins), including proteins protease inhibitors, natural protease inhibitors, and synthetic protease inhibitors. (1). Antiprotozoal activity: protease inhibitors could be used against malaria and gastrointestinal protozoal infections; (2). Antiretrovirals: protease inhibitors were the second class of antiretroviral drugs developed widely used to treat HIV/AIDS and hepatitis C; (3). Anticancer activity: Researchers are investigating whether protease inhibitors could possibly be used to treat cancer. For example, nelfinavir and atazanavir are able to kill tumor cells in culture. Inhibitors of the proteasome, such as bortezomib are now front-line drugs for the treatment of multiple myeloma. Marimastat and batimastat are two of the matrix metalloproteinase inhibitors that can be used to treat cancer.
The Protease Inhibitor Library by TargetMol®, containing 295 small protease and proteasome inhibitors, can be used for research in Chemical Genomics and drug screening.

Pack Size		Price
100 μL * 10 mM (in DMSO)	USD	6,430.00
250 μL * 10 mM (in DMSO)	USD	10,606.00
1 mg	USD	10,606.00

Serotonin Receptor-Targeted Compound Library

Catalog No. L2800 — 170 compounds

Serotonin or 5-hydroxytryptamine (5-HT) is a monoamine neurotransmitter, a derivative from the amino acid tryptophan, and mainly located in the enterochromaffin cells in the GI tract and central nervous system (CNS). It has a popular image as a contributor to feelings of well-being and happiness, though its actual biological function is complex and multifaceted, modulating cognition, reward, learning, memory, and numerous physiological processes. Serotonin receptors, are a group of G protein-coupled receptor and ligand-gated ion channels found in the central and peripheral nervous systems. They can be divided into 7 families of G protein-coupled receptors except for the 5-HT3 receptor, a ligand-gated ion channel, which activates an intracellular second messenger cascade to produce an excitatory or inhibitory response. They mediate both excitatory and inhibitory neurotransmission, influencing various biological and neurological processes. The serotonin receptors are the target of a variety of pharmaceutical and recreational drugs, including many antidepressants, antipsychotics, anorectics, antiemetics, gastroprokinetic agents, antimigraine agents, hallucinogens, and entactogens.
The Serotonin Receptor-Targeted Compound Library by TargetMol®, collecting 170 small chemicals targeting serotonin receptors, can be used for high throughput screening and high content screening, and drug discovery in neurological disorders.

Pack Size		Price
100 μL * 10 mM (in DMSO)	USD	2,737.00
250 μL * 10 mM (in DMSO)	USD	4,566.00
1 mg	USD	4,566.00

Sodium Channel Blocker Library

Catalog No. L7400 — 62 compounds

Sodium channels are integral membrane proteins that form ion channels, conducting sodium ions (Na+) through a cell's plasma membrane. According to the trigger that opens the channel for such ions, they can be classified into Voltage-gated sodium channels and ligand-gated sodium channels. Sodium channels are highly selective for the transport of sodium ions across cell membranes. In excitable cells such as neurons, myocytes, and certain types of glia, sodium channels are responsible for the rising phase of action potentials. Many of the most common neurological disorders, such as epilepsy, migraine, neurodegenerative diseases, and neuropathic pain, involve abnormalities of neuronal excitability. There is a growing body of data that implicates abnormal expression and function of voltage-gated sodium channels (VGSCs) in these disorders.
Pharmacological inhibitors of VGSCs have been used for decades to treat epileptic seizures, the most common disease of neuronal excitability, and arrhythmia, and it is becoming increasingly evident that these antiepileptic VGSC blockers might also be efficacious against a broad range of neurological disorders. Sodium channels serve as specific targets for a large variety of chemically distinct neurotoxins produced by many different animals and plants. The development of drugs with enhanced selectivity for specific VGSC isoforms might be an effective and novel approach for the treatment of several neurological diseases.
TargetMol®'s Sodium Channel Blocker Library collects 62 reported sodium channel blockers and agonists, and is an ideal tool for screening more selective and efficient drugs targeting potassium channels.

Pack Size		Price
100 μL * 10 mM (in DMSO)	USD	1,350.00
250 μL * 10 mM (in DMSO)	USD	2,290.00
1 mg	USD	2,290.00

TGF-beta/Smad Compound Library

Catalog No. L4100 — 116 compounds

Members of the transforming growth factor-β (TGF-β) family control growth, differentiation and apoptosis of cells, and have important functions during embryonic development. There are three known isoforms of TGF-β (TGF-β1, TGF-β2 and TGF-β3) expressed in mammalian tissues. TGF-β isoforms signal through three surface receptors, known as the TGF-β type I, type II, and type III receptors (TβRI, TβRII, and TβRIII, respectively) which are expressed on the surface of many cell types such as fibroblasts, lymphocytes, and hemopoietic cells, etc. The binding of TGF-β and receptors transduces the signals by phosphorylating carboxy-terminal serine residues of receptor-regulated (R-) Smads. The activated R-Smads form hetero-oligomeric complexes with a common-partner (co-) Smad, that is, Smad4 in vertebrate cells. The complexes translocate into the nucleus where they regulate the expression of target genes.
TGF-beta/Smad Compound Library from TargetMol®, a unique collection of 116 TGF-beta/Smad signaling targeted compounds, can be used for research in TGF-beta/Smad signaling and related drug screening (high throughput and high content screening).

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	1,920.00
250 µL * 10 mM (in DMSO)	USD	3,211.00
1 mg	USD	3,211.00

Tyrosine Kinase Inhibitor Library

Catalog No. L2200 — 640 compounds

A protein kinase is a kinase enzyme that modifies other molecules, mostly proteins, by chemically adding phosphate groups to them (phosphorylation) to regulate the majority of cellular pathways, especially those involved in signal transduction. Phosphorylation usually results in a functional change of the target protein (substrate) by changing enzyme activity, cellular location, or association with other proteins. Of the 518 known kinases, the most successful class for drug targeting is the tyrosine kinase family consisting of 90 distinct and diverse members. Abnormal expression of PTK usually leads to cell proliferation disorders, and is closely related to tumor invasion, metastasis and tumor angiogenesis. More recently, PTKs played a pivotal role in inflammatory diseases such as idiopathic pulmonary fibrosis.
The Tyrosine Kinase Inhibitor Library by TargetMol®, containing 640 tyrosine kinase inhibitors, can be used for research in tyrosine kinase signaling, and drug screening for related diseases.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	10,661.00
250 µL * 10 mM (in DMSO)	USD	17,576.00
1 mg	USD	17,576.00

Ubiquitination Compound Library

Catalog No. L8600 — 160 compounds

Ubiquitination involves covalent attachment of ubiquitin, a small 8-kDa protein, to a substrate and results in recognition and shuttling of the substrate to the 26S proteasome complex for degradation. Ubiquitination, the structured degradation and turnover of cellular proteins, is regulated by the ubiquitin–proteasome system (UPS). The ubiquitination process is tightly controlled by three families of enzymes: ubiquitin-activating enzymes (E1s), ubiquitin-conjugating enzymes (E2s), and finally ubiquitin ligases (E3s). Ubiquitination affects cellular processes (apoptosis, cell cycle, DNA damage repair, and membrane transportation, etc.) by regulating the degradation of proteins (via the proteasome and lysosome), coordinating the cellular localization of proteins, activating and inactivating proteins, and modulating protein-protein interactions. The ubiquitin pathway has been implicated in the pathogenesis of several diseases and genetic disorders: cancer, cardiovascular disease, and neurodegenerative disorders, etc. Recent advances in our understanding of the role and molecular mechanisms of UPS components in disease – mainly DUBs and E3 ligases, the development of high-quality chemical tools and novel inhibitors, as well as preclinical studies demonstrating chemical tractability and therapeutic potential – have dramatically taken the ubiquitin-proteasome system from an improbable target class, to one of the most robust and exciting arenas for the discovery of novel drugs.
TargetMol®'s Ubiquitination Compound Library collects 160 ubiquitination-related small molecules, targeting proteasome, E1/E2/E3 Enzyme, DUB, p97, etc.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	3,200.00
250 µL * 10 mM (in DMSO)	USD	4,800.00
1 mg	USD	4,800.00

Wnt/Hedgehog/Notch Compound Library

Catalog No. L4300 — 136 compounds

The Wnt signaling pathway is an ancient and evolutionarily conserved pathway that regulates crucial aspects of cell fate determination, cell migration, cell polarity, neural patterning and organogenesis during embryonic development. Aberrant regulation of the Wnt signaling pathway is prevalent in cancer biology. The Hedgehog (Hh) pathway is a major regulator of many fundamental processes in vertebrate embryonic development including stem cell maintenance, cell differentiation, tissue polarity and cell proliferation. Constitutive activation of the Hh pathway leading to tumorigenesis is seen in basal cell carcinomas and medulloblastoma. A variety of other human cancers, including brain, gastrointestinal, lung, breast and prostate cancers, also demonstrate inappropriate activation of this pathway. Targeting the Hh signaling pathway provides a new and exciting therapeutic option for a wide variety of cancers. The Notch signaling pathway is a highly conserved cell signaling system present in most multicellular organisms. The Notch signaling cascade is critical for cell proliferation, differentiation, development and homeostasis. Deregulated Notch signaling is found in various diseases, such as T-cell leukemia, breast cancer, prostate cancer, colorectal cancer and lung cancer as well as central nervous system (CNS) malignancies, CADASIL, Alagille syndrome, spondylocostal dysostosis, etc.
Wnt/Hedgehog/Notch Compound Library from TargetMol®, a unique collection of 136 Wnt/Hedgehog/Notch signaling targeted compounds, can be used for research in Wnt/Hedgehog/Notch signaling and related drug screening (high throughput and high content screening).

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	2,420.00
250 µL * 10 mM (in DMSO)	USD	3,944.00
1 mg	USD	3,944.00

Characteristic Bioactive Libraries

Antibiotics Library

Catalog No. L4400 — 680 compounds

Antibiotics are used to treat or prevent bacterial infections, and sometimes protozoan infections, having saved thousands of lives. The discovery and application of antibiotics added 5-10 years to the life expectancy of the average American; therefore, it is recognized as one of the greatest medical advances of the 20th century. However, inappropriate antibiotic treatment and overuse of antibiotics have contributed to the emergence of antibiotic-resistant bacteria. Antibiotic resistance is increasing globally and fast because of greater access to antibiotic drugs in developing countries, and it is now a major threat to public health, economic growth, and global stabilization. Therefore, it is an urgent need to develop new drugs targeted at resistant organisms while limiting antibiotic use.
The TargetMol®'s Antibiotics Library, a focused collection of 680 compounds with antibiotic activity, can be used for antibacterial research and related drug screening.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	11,294.00
250 µL * 10 mM (in DMSO)	USD	17,042.00
1 mg	USD	17,042.00

Beta-Lactam Compound Library

Catalog No. L9820 — 90 compounds

β-lactam compounds are compounds that contain a beta-lactam ring in their molecular structure. This includes penicillin derivatives (penams), cephalosporins (cephems), monobactams, carbapenems and carbacephems. Most β-lactam antibiotics work by inhibiting cell wall biosynthesis in the bacterial organism and are the most widely used group of antibiotics. Until 2003, when measured by sales, more than half of all commercially available antibiotics in use were β-lactam compounds.
TargetMol®'s Beta-Lactam Compound Library collects 90 beta-lactam compounds with annotated activities, which can be used for research in antibacterial and anti-infection.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	1,607.00
250 µL * 10 mM (in DMSO)	USD	2,673.00
1 mg	USD	2,673.00

Bioactive Compound Library

Catalog No. L4000 — 8829 compounds

Product Description

It contains more than 8829 small molecule compounds, with known biological activities causing biological reactions in cells, tissue even the whole body, including Clinical compound library (L3400), Preclinical compound library (L3410), and Approved drug library (L1000). All compounds have clear targets and detailed descriptions of the key points to drug research and development like drug repurposing, small molecule inducing stem cell differentiation, and target identification in mechanism interrogation.
Many scientists have identified small molecules that can regulate cell fate and function, and stem cell differentiation by screening annotated bioactive compound library with confirmed activity and known targets. Recent advances in iPSC technology have made reprogramming of somatic cells towards pluripotency possible and simpler. Using both phenotypic screening and hypothesis-driven approaches, a growing number of compounds have been identified that can functionally replace reprogramming transcription factors, enhance the efficiency of iPSC generation and accelerate the reprogramming process by single-use or a combination of several molecules with success in cardiomyocyte differentiation and proliferation, neural progenitor cells, etc.
In the library, we provide the peptides and other drug molecules with low solution stability in the form of dry powder (set as Part B) in order to ensure the best using-effect of the compound library and increase the probability of successful screening as much as possible.

Product Advantage

- A unique collection of 8829 small molecule compounds with validated activity for high throughput screening(HTS), high content screening(HCS), cell induction, and target identification;
- All compounds have clear target information;
- An effective tool for discovering drug repurposing, cell induction, and new drug target screening;
- Covers various disease research areas, such as Cancer, Metabolism, Immunology and Cardiovascular system, etc;
- NMR and HPLC/LCMS validated to ensure high purity and quality and reduce false-positive rate.

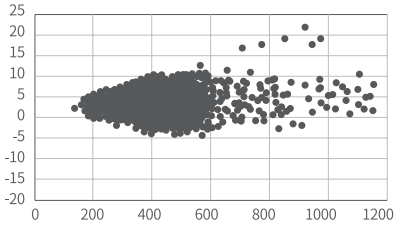
Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	65,982.00
250 µL * 10 mM (in DMSO)	USD	109,966.00
1 mg	USD	109,966.00

Drug-Like Properties

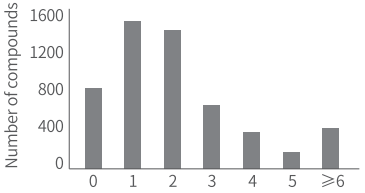
% of compounds compliant with Lipinski' s Rules

PhysChem Properties	% Compounds
<5 H-Bond donors	89
<10 H-Bond acceptors	89
cLogP<5	89
MW<500	80

cLogP vs MW

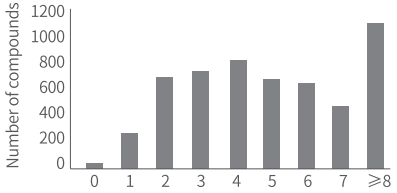


Distribution of HB Donors



HB Donor

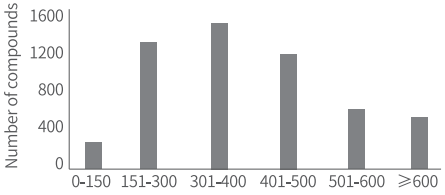
Distribution of HB Acceptors



HB Acceptor

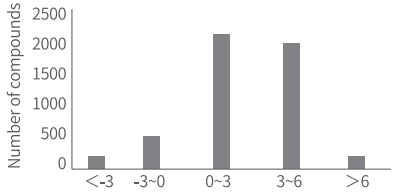
Drug-Like Properties

Distribution of Molecular Weight



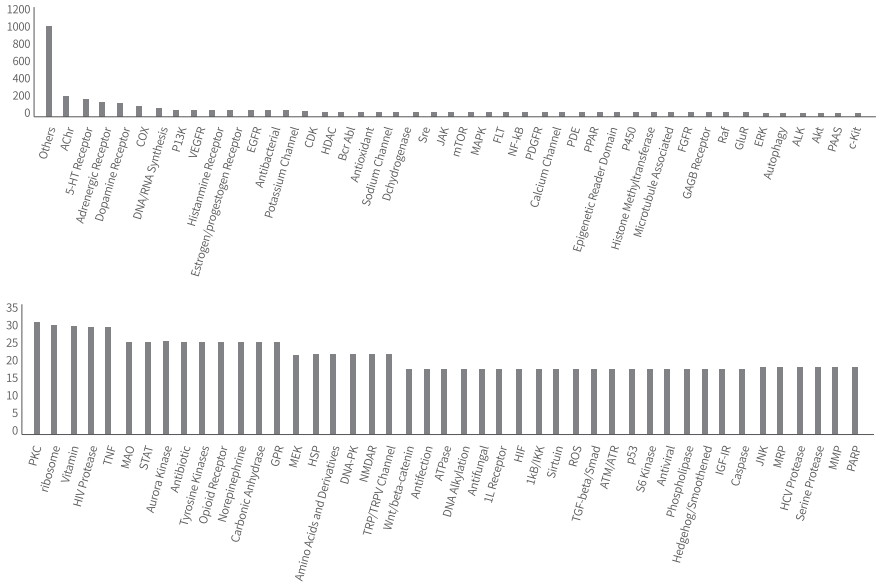
Molecular Weight

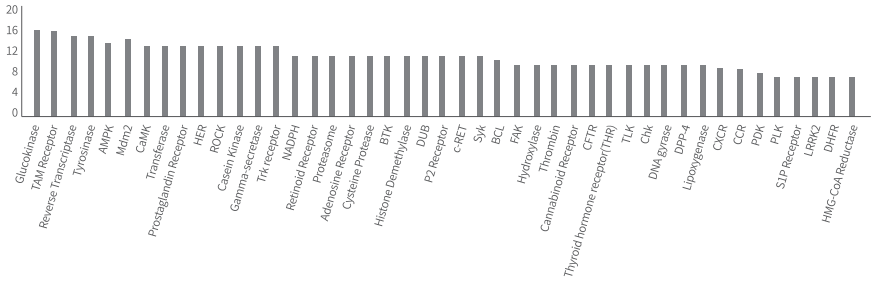
Distribution of cLogP



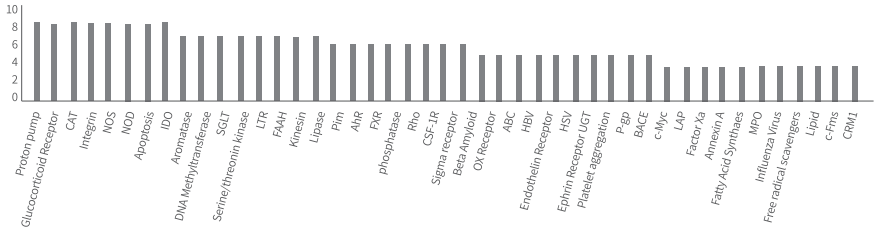
cLogP

Target Composition

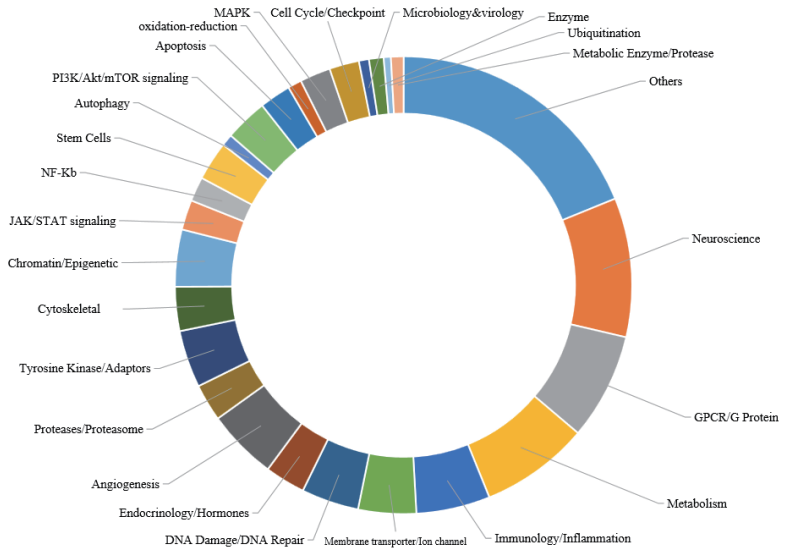




Target Composition



Signaling Pathways



Featured Novel Bioactive Compound Library

Catalog No. L4150 — 990 compounds

It is well-selected from Novel Bioactive Compound Library (D7800), from which 1-15 compounds with the highest scores (activity value, pharmacological properties, structure-diversity, etc.) were chosen. This library consists of 990 compounds without compromising the number of targets, but with more unique structures than known drugs and more bioactivity information than drug-like compounds. It is supposed to help generate a higher hit rate, and is a powerful compound library for drug discovery and target identification.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	8,174.00
250 µL * 10 mM (in DMSO)	USD	12,489.00
1 mg	USD	12,489.00

Bioactive Lipid Compound Library

Catalog No. L7000 — 385 compounds

Bioactive lipids have been shown to provide health benefits either through modification of tissue fatty acid composition or induction of cell signaling pathways, due to their pivotal role in immune regulation, inflammation, and maintenance of tissue homeostasis. While some health benefits are derived from the consumption of short to medium-chain fatty acids, evidence suggests that the polyunsaturated fatty acids (PUFAs) are the most important bioactive lipids. PUFAs are found mostly in plant seed oils and are important substrates for the biosynthesis of cellular hormones (eicosanoids) and other signaling compounds that modulate human health. The beneficial health effects of PUFAs seem to be dependent on their isomer configuration as the cis-isomer is the predominant bioactive form that enhances membrane fluidity when incorporated into cells. Increased membrane fluidity enhances cell to cell communication and helps maintain normal homeostasis or prevent the development of metabolic disorders.
The TargetMol®'s Bioactive Lipid Inhibitor Library, a unique collection of 385 bioactive lipids-related compounds, can be used for research in bioactive lipids, and high throughput screening (HTS) and high content screening (HCS).

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	6,428.00
250 µL * 10 mM (in DMSO)	USD	10,725.00
1 mg	USD	10,725.00

Cardiotoxicity Compound Library

Catalog No. L4900 — 132 compounds

Cardiotoxicity is one of the leading causes of drug attrition during development, and accounts for 22-28% of US post-marketing drug withdrawal. Therefore, developing sensitive in vitro assays assessing drug-induced cardiotoxicity in preclinical and early clinical stages is especially important for drug development.
The TargetMol®'s Cardiotoxicity Compound Library, a unique collection of 132 cardiotoxicity inducing compounds, can be used for chemical toxicity evaluation and prediction.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	2,183.00
250 µL * 10 mM (in DMSO)	USD	3,672.00
1 mg	USD	3,672.00

Chromatin Modification Compound Library

Catalog No. L8300 — 256 compounds

Chromatin modification, also called Chromatin remodeling, is the rearrangement of chromatin from a condensed state to a transcriptionally accessible state, allowing transcription factors or other DNA binding proteins to access DNA and control gene expression. Such remodeling is principally carried out by 1) covalent histone modifications by specific enzymes, e.g., histone acetyltransferases (HATs), deacetylases, methyltransferases, and kinases, and 2) ATP-dependent chromatin remodeling complexes which either move, eject or restructure nucleosomes. Chromatin remodeling is highly implicated in epigenetics. Epigenetic modifications to histone proteins such as methylation/demethylation and acetylation/deacetylation can alter the structure of chromatin resulting in transcriptional activation or repression. Aberrations in chromatin remodeling proteins are found to be associated with human diseases, including cancer. Targeting chromatin remodeling pathways is currently evolving as a major therapeutic strategy in the treatment of several cancers.
Chromatin Modification Compound Library from TargetMol® is a unique collection of 256 compounds targeting chromatin remodeling pathways that can be used for high throughput and high content screening.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	5,290.00
250 µL * 10 mM (in DMSO)	USD	8,832.00
1 mg	USD	8,832.00

CNS-Penetrant Compound Library

Catalog No. L5900 — 516 compounds

The blood–brain barrier (BBB) is a highly selective semipermeable border that separates the circulating blood from the brain and extracellular fluid in the central nervous system (CNS). In its neuroprotective role, the blood–brain barrier functions to hinder the delivery of many potentially important diagnostic and therapeutic agents to the brain. Overcoming the difficulty of delivering therapeutic agents to specific regions of the brain presents a major challenge to the treatment of most brain disorders. Choosing the compounds that could penetrate BBB into the compound library targeting CNS is critical for CNS drug discovery. Based on the scientific literature, TargetMol® collects 516 out of 5000 compounds as CNS-Penetrant Compound Library, which can be used for CNS-Penetrant related research and drug screening for CNS diseases.

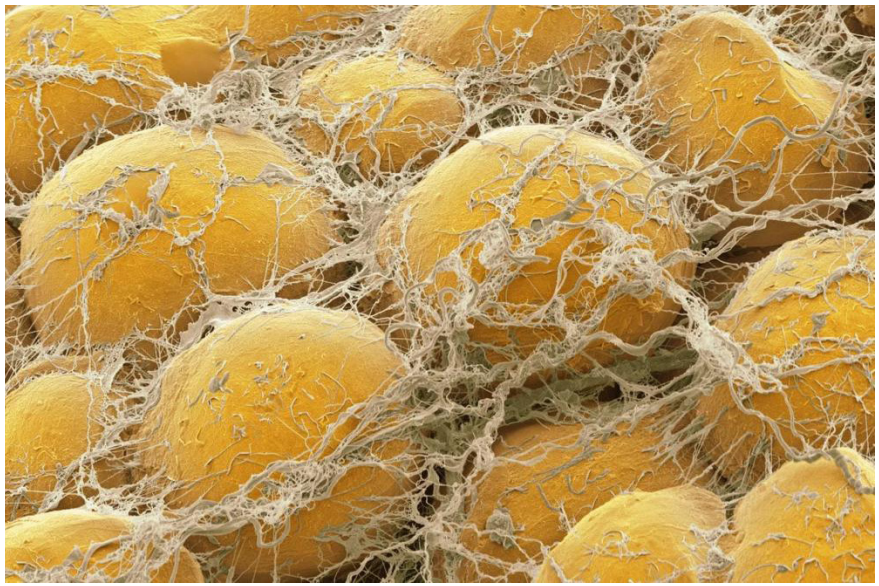
Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	8,588.00
250 µL * 10 mM (in DMSO)	USD	14,110.00
1 mg	USD	14,110.00

Coagulation and Anticoagulation Compound Library

Catalog No. L7500 — 154 compounds

Coagulation is the process by which blood changes from a liquid to a gel, forming a blood clot. Substances that take part in the coagulation cascade are called clotting factors. The blood clotting process is complex and mainly involves three steps: prothrombin activator being produced, prothrombin being converted to thrombin, and fibrinogen being converted to fibrin. Anticlotting mechanisms are important in restricting clot formation to the site of injury. The two major systems are the anticoagulant and fibrinolytic systems. The balance of coagulation and anticlotting mechanisms keeps the hemostatic system functioning efficiently. It is currently believed that the anticoagulant mechanism mainly has the barrier function of vascular endothelium, fibrin adsorption, phagocytosis of mononuclear macrophage system and physiological anticoagulant substances.
The TargetMol®'s Procoagulants and Anticoagulants Library has a unique collection of 154 procoagulation and anticoagulation related compounds, which can be used for research in coagulation and anticoagulation mechanisms, and related drug development.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	2,450.00
250 µL * 10 mM (in DMSO)	USD	4,437.00
1 mg	USD	4,437.00



Covalent Inhibitor Library

Catalog No. L9410 — 943 compounds

Covalent inhibitors are small organic molecules that interact with specific target proteins and form a covalent bond, resulting in an alteration of the protein conformation and subsequently inhibiting the protein activity. With some exceptions, protein modification by covalent inhibitors is usually irreversible. Covalent inhibitors possess significant advantages over non-covalent inhibitors, such that covalent warheads can target rare residues of a particular target protein, thus leading to the development of highly selective inhibitors and achieving a more complete and continued target occupancy in living systems. However, toxicity can be a real challenge related to this class of therapeutics due to their potential for off-target reactivity and has led to these drugs being disfavored as a drug class. Consequently, there has been a reluctance to apply a covalent mode of action in drug discovery programs and avoided by the pharmaceutical industry.

Although the majority of successful covalent drugs were discovered through serendipity in phenotypic screens, and their molecular mechanisms were elucidated afterward, covalent drugs have made a major impact on human health and have been highly successful drugs for the pharmaceutical industry over the last 100 years, such as penicillin, omeprazole, clopidogrel, aspirin, fluorouracil, and third generation of irreversible EGFR tyrosine kinase inhibitor AZD9291/Osimertinib.

In recent years, the distinct strengths of covalent inhibitors in overcoming drug resistance have been recognized. It appears that irreversible inhibitors may maintain activity against drug-resistant mutations that are acquired after treatment with reversible inhibitors. Irreversible inhibition has important and potentially advantageous consequences for drug pharmacodynamics in which the level and frequency of dosing relates to the extent and duration of the resulting pharmacological effect. The unique pharmacodynamic feature of covalent inhibitors might bring certain practical advantages. The prolonged duration of drug action on the target effectively uncouples the pharmacodynamics of the drug from the pharmacokinetics of exposure, as target inhibition persists after the drug has been cleared. This property of covalent drugs enables less frequent dosing and the potential for lower drug doses. In addition, more and more studies have found that many major diseases, such as malignant tumors, are regulated by kinases, and these enzymes have also become the most attractive drug targets. Over the past decade, covalent kinase inhibitors (CKI) have seen a resurgence in drug discovery. Current FDA-approved CKIs will bring the dawn to cancer chemotherapy. The drug design and optimization of covalent inhibitors have become a hot spot in drug discovery.

The irreversible covalent inhibitor molecule is divided into two parts: a seeker and a warhead. After entering the body, the seeker and the target protein binding site first form a non-covalent interaction, and then the warhead forms an irreversible covalent bond with the nucleophilic residues of target protein. Common warheads include Michael acceptors, Sulfonyl fluoride, disulfide bond, etc.

The structure and mechanism of reversible covalent inhibitors are similar to irreversible covalent inhibitors, but the difference is that the covalent binding to the target protein is reversible. The warheads for reversible covalent inhibitors are reversible nucleophilic addition reaction receptors such as cyano group and ketone carbonyl group. The reversibility of its covalent binding to the target makes its pharmacokinetics fall in between irreversible covalent inhibitors and non-covalent inhibitors. To a certain extent, reversible covalent inhibitors share the advantages of irreversible covalent inhibitors in the prolonged duration of action and the potential for lower drug doses, while reducing the risk of toxicity caused by off-target.

TargetMol® collects 943 small molecules including identified covalent inhibitors and other molecules having covalent reactive groups as warheads, such as chloroacetyl，2-Chloropropionyl，Acryloyl，alkyne，sulfonyl fluoride, acrylamide, ketocarbonyl，disulfide bond, etc.

Pack Size		Price
100 μL * 10 mM (in DMSO)	USD	15,711.00
250 μL * 10 mM (in DMSO)	USD	25,921.00
1 mg	USD	25,921.00

DNA Damage and Repair Compound Library

Catalog No. L3900 — 773 compounds

A significant barrier to effective cancer therapy is the development of resistance to the drugs utilized, therefore, identifying new biological targets and designing new drugs becomes one of the most important strategies. Among the various potential targets, DNA damage and repair system in cancer cells is one of the most pivotal targets. The use of unspecific antibiotics to treat bacterial infections has caused a great deal of multiple resistant strains making the current antibiotics therapies less effective. Developing inhibitors of DNA repair and related pathways in pathogens will have utility in the treatment of infections.

The TargetMol®'s DNA Damage & Repair Compound Library, a unique collection of 773 DNA Damage & Repair related compounds, can be used for research in DNA damage and repair, and high throughput screening (HTS) and high content screening (HCS).

Pack Size		Price
100 μL * 10 mM (in DMSO)	USD	19,860.00
250 μL * 10 mM (in DMSO)	USD	29,503.00
1 mg	USD	29,503.00

DNA Damage and Repair Compound Library Plus

Catalog No. L3980 — 667 compounds

A significant barrier to effective cancer therapy is the development of resistance to the drugs utilized, therefore, identifying new biological targets and designing new drugs becomes one of the most important strategies. Among the various potential targets, DNA damage and repair system in cancer cells is one of the most pivotal targets. The use of unspecific antibiotics to treat bacterial infections has caused a great deal of multiple resistant strains making the current antibiotics therapies less effective. Developing inhibitors of DNA repair and related pathways in pathogens will have utility in the treatment of infections.

TargetMol®'s DNA Damage and Repair Compound Library Plus, a unique collection of 667 DNA Damage & Repair related compounds, covering 19 various DNA damage & repair targets with IC50 less than 3 μM, can be used for research in DNA damage and repair, and high throughput screening (HTS) and high content screening (HCS).

Pack Size		Price
100 μL * 10 mM (in DMSO)	USD	9,944.00
250 μL * 10 mM (in DMSO)	USD	16,903.00
1 mg	USD	16,903.00

Drug-Induced Liver Injury (DILI) Compound Library

Catalog No. L5510 — 939 compounds

Adverse drug events such as cardiotoxicity, hepatotoxicity and other organ toxicities, keep surfacing in the clinic and idiosyncratic drug toxicity continues to haunt the drug development process. Drug-induced liver injury (DILI) is common and nearly all classes of medications can cause liver disease. Although cardiotoxicity remains one of the main reasons for drug development termination, both during preclinicall and clinical stages, DILI is the most common reason cited for withdrawal of an approved drug. The reason for this most likely lies in the fact that significant advancement in understanding the mechanistic basis of cardiotoxicity but the imperfect prediction of DILI risk.
DILI is thought to occur via several different mechanisms. Among these are direct impairment of the structural and functional integrity of the liver (e.g., mitochondrial dysfunction); production of a metabolite that alters hepatocellular structure and function; production of a reactive drug metabolite that binds to hepatic proteins to produce new antigenic drug-protein adducts, which are targeted by hosts' defenses (the hapten hypothesis); and initiation of a systemic hypersensitivity response (i.e., drug allergy) that damages the liver.
TargetMol®'s Drug-induced Liver Injury Compound Library collects 939 hepatotoxicity causing compounds, including anticancer drugs, antibiotics, antituberculosis agents, antiretrovirals, antiepileptic agents, and cardiac medications, etc. It is not only a powerful tool for DILI research and other drug toxicities but is of crucial value in understanding the mechanisms of DILI, identifying biomarkers for early DILI prediction, and allowing timely recognition during drug development, thus finally achieving successful DILI prevention and assessment in the pre-marketing phase.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	14,077.00
250 µL * 10 mM (in DMSO)	USD	23,372.00
1 mg	USD	23,372.00

Endocrinology-Hormone Compound Library

Catalog No. L2400 — 681 compounds

Endocrine glands are made of a group of cells that secrete their products, hormones, directly into the blood rather than through a duct. Hormones are transported by the circulatory system to target distant organs to regulate physiology and behavior, such as metabolism, growth, development, and reproduction. Hormones have diverse chemical structures, mainly of 3 classes: eicosanoids, steroids, and amino acid/protein derivatives. Endocrine disease is characterized by irregulated hormone release, inappropriate response to signaling, lack of a gland, or structural enlargement in a critical site such as the thyroid.
The Endocrinology-Hormone Compound Library by TargetMol®, containing 681 compounds targeting endocrine system, can be used for research in endocrine system, high throughput screening and high content screening for new drugs in endocrine diseases.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	10,945.00
250 µL * 10 mM (in DMSO)	USD	18,267.00
1 mg	USD	18,267.00

Fluorochemical Library

Catalog No. L5100 — 586 compounds

Fluorine atoms have a unique combination of electronic and physical properties. As such, when incorporated into active pharmaceutical ingredients (APIs), fluorine atoms often influence their protein binding affinity and lipophilicity but not the shape of the resulting fluorochemicals. Fluorination can thus significantly impact the bioavailability or metabolic stability of drug substances. The pivotal role that the element fluorine plays in modulating the properties of bioactive molecules is reflected by the growth of its presence in approved drugs, as evidenced by the fact that between 15% to 20% of all medicines and agrochemicals on the market contain at least one fluorine atom in their structure. As of 2009, the FDA had approved >140 fluorine-containing drugs, such as fluorouracil, Miglitol, Gemcitabine, Sofosbuvir, atorvastatin, fluoxetine, ciprofloxacin, etc.
The judicious introduction of fluorine into a molecule can productively influence conformation, pKa, intrinsic potency, membrane permeability, metabolic pathways, and pharmacokinetic properties.
Nowadays, the application of specialty fluorochemicals in the pharmaceutical industry has been increasingly widespread. TargetMol®'s fluorochemical library has become an effective tool for developing new anticancer drugs, anesthetics, antidepressants, antifungals, antiviral drugs, antibiotics, cholesterol-lowering agents, and anti-inflammatory agents. In addition, in agricultural uses, the addition of fluorine to many agricultural herbicides, pesticides, and fungicides improves the potency and therefore reduces the required application rate of these substances.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	9,745.00
250 µL * 10 mM (in DMSO)	USD	16,184.00
1 mg	USD	16,184.00

Glutamine Metabolism Compound Library

Catalog No. L2550 — 455 compounds

L-glutamine is a non-essential amino acid that is often simply called glutamine. It is produced by the body. Glutamine is synthesized from NH4+ and glutamate. The conversion of glutamate to glutamine is regulated by glutamine synthetase (GS) and is a key step in nitrogen metabolism. Although normally synthesized in adequate amounts, endogenous glutamine production may be inadequate during periods of metabolic stress or under the condition of disease.
Glutamine is crucial for many metabolic functions, including protein and glutathione synthesis, energy production, maintenance of optimal antioxidant status, and immune function. Glutamine is the main metabolic substrate of macrophages and important for the function of macrophages; Glutamine is an important biosynthetic precursor for amino acid, protein and nucleic acid synthesis; Glutamine serves as a source of fuel for the cells lining the intestines, and without it, these cells may waste away; Glutamine is significantly involved in the synthesis of glutathione, a very important intracellular antioxidant and detoxication factor.
Cancer cells undergo a reprogramming of metabolism in order to maintain bioenergetics, redox status, cell signaling and biosynthesis, in a oftenly poorly vascularized, nutrient-deprived microenvironment. A metabolic characteristic of many cancer cells is a dependence on an exogenous supply of glutamine, exhibiting “glutamine addiction”. Glutamine enters the cell through the amino acid transporter, ASCT2/SLC1A5, and is converted to glutamate in the mitochondria through a deamination reaction catalyzed by glutaminase (GLS). Glutamate is converted to the TCA cycle intermediate α-ketoglutarate (α-KG) by either glutamate dehydrogenase (GDH) or by the alanine or aspartate transaminases (TAs), which produce their corresponding amino acid in addition to α-KG, a process termed glutaminolysis. Humans express 4 isoforms of glutaminase which is the restriction and initiation enzyme in the glutaminolytic pathway. GLS encodes 2 types of kidney-type glutaminase with a high activity and low Km. GLS2 encodes 2 forms of liver-type glutaminase with a low activity and allosteric regulation.
Glutamine coordinates intracellular signaling to promote cancer growth in addition to acting as an important substrate for carbon and nitrogen production. For example, MYC transcriptionally represses miR-23a/b, leading to higher expression of mitochondrial glutaminase. Glutamine stimulates mTORC1 activity and in turn, impairs autophagy initiation through the negative regulation of ULK1 by several mechanisms. Thus, intervention in glutamine metabolic processes could provide novel approaches to improve cancer treatment.
TargetMol® owns a unique collection of 455 compounds targeting the main proteins and enzymes involved in the glutamine metabolism pathway. Glutamine Metabolism compound library is a useful tool for research in glutamine metabolic processes and drug discovery.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	7,400.00
250 µL * 10 mM (in DMSO)	USD	14,490.00
1 mg	USD	14,490.00

Glycometabolism Compound Library

Catalog No. L2520 — 638 compounds

Glucose and glycogen are initial materials involved in glycometabolism. A chronically irregular diet could result in the disorders of glycometabolism, which was manifested by the gradual deterioration of glucose tolerance over time, leading to increased fasting blood glucose or impaired glucose tolerance. The clinical manifestations of glycometabolism-related disorder are hyperglycemia or hypoglycemia, which might eventually contribute to some serious diseases, such as diabetes, G6PD deficiency, obesity and malnutrition. In addition, favored glycolysis under aerobic conditions (aerobic glycolysis), or the Warburg effect, the transition from oxidative phosphorylation to glycolysis, accompanied by the accumulation of lactate by-products in the surrounding microenvironment and 20-30 times faster rate of glucose metabolism than the complete oxidation of glucose in the mitochondria, represents the most typical change observed in the metabolism of cancer cells. Therefore, a key to selective killing of cancer cells lies in their dependence on glycolysis. Targeting tumor cell metabolism has become a successful approach to the prevention or treatment of cancer. Most efforts have focused on the use of small molecules to inhibit the function of metabolic enzymes, which has been comprehensively reviewed elsewhere. Increasing evidence supports many glycolytic enzymes and transporters as candidates for cancer treatment.
TargetMol®'s Glycometabolism Compound Library collects 638 glycometabolism-related compounds, targeting GLUTs, Hexokinase（HK）, Pyruvate Kinase（PK）, phosphofructokinase（PFK）, IDH1/2, LDH, AMPK, etc. It is a powerful tool for research in glycometabolism-related disorders and cancer.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	10,374.00
250 µL * 10 mM (in DMSO)	USD	17,370.00
1 mg	USD	17,370.00

Gut Microbial Metabolite Library

Catalog No. L2540 — 352 compounds

The gut microbiome in humans can be considered as an organ, which has functions critical for human metabolism, digestion, maintenance of gut barrier function and immunomodulation. Human metabolism is highly associated with altered microbiota composition.
Moreover, the gut microbiome has been linked to many diseases not classically associated with microbes, such as metabolic diseases including obesity and obesity-related complications such as nonalcoholic fatty liver disease (NAFLD), insulin resistance and type 2 diabetes mellitus (T2DM), rheumatoid arthritis and psychiatric disorders. The gastrointestinal (GI) tract is considered the largest immunological organ in the body having a central role in regulating immune homeostasis, relying on the dynamic interactions between intestinal epithelial cells, immune cells and microbiome in shaping specific immune responses to antigens. The gut microbiota contributes to host physiology through the production of a myriad of metabolites. These metabolites exert their effects within the host as signaling molecules（“messengers”）and substrates for metabolic reactions, such as influencing human energetics, suppressing inflammation through distinct mechanisms, regulating intestinal epithelial cell homeostasis, immune cell response, and neuronal excitability, etc. Therefore, the study on gut microbial metabolites will be helpful in discovering the mechanisms of some diseases and developing appropriate and effective therapies.
TargetMol®'s Gut Microbial metabolite Library collects 352 gut microbial metabolites which can be used in research of gut microbiome and its related drug development.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	5,859.00
250 µL * 10 mM (in DMSO)	USD	9,623.00
1 mg	USD	9,623.00

Hematopoietic Toxicity Compound Library

Catalog No. L3100 — 104 compounds

The TargetMol®'s Hematopoietic Toxicity Compound Library is a focused collection of 104 compounds with defined and diverse hematopoietic toxicity, including myelosuppression, neutropenia, leukopenia, anemia, and many more. The bioactivities of all compounds were confirmed by bioassays and reported by scientific literature. Some of them are FDA-approved. The library is an essential tool for predictive toxicology screening and assay development.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	1,480.00
250 µL * 10 mM (in DMSO)	USD	2,790.00
1 mg	USD	2,790.00

Histone Modification Compound Library

Catalog No. L3500 — 194 compounds

A histone modification is a covalent post-translational enzymatic modification to histone proteins which includes methylation, phosphorylation, acetylation, ubiquitylation, and sumoylation. Histone modification impacts gene expression by altering chromatin structure or recruiting histone modifiers. Therefore, histone modifications act in diverse biological processes such as transcriptional activation/inactivation, chromosome packaging, and DNA damage/repair. Thus, quantitative detection of various histone modifications would provide useful information for a better understanding of epigenetic regulation of cellular processes and the development of histone modifying enzyme-targeted drugs.
The TargetMol®'s Histone Modification Compound Library, a unique collection of 194 histone modification related compounds, can be used for research in histone modification and related drug screening.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	3,104.00
250 µL * 10 mM (in DMSO)	USD	5,626.00
1 mg	USD	5,626.00

Human Endogenous Metabolite Library

Catalog No. L2500 — 910 compounds

Product Description

Changes in biological status (such as hypoxia, nutrients, drugs) usually cause the perturbations in the concentrations and fluxes of specific endogenous metabolites involved in a number of key disease-related or other specific cellular pathways. Extensive efforts in recent years have been focused on metabolic alterations in cancer, the products of intermediary metabolism have been a topic of considerable research interest. Cancer cells exhibit profound alterations in their metabolism. The quantitative measurement of the dynamic multiparametric metabolites, identification and quantification of intermediary metabolism can better help predict the tumor progress, understand the metabolic pathways and molecular mechanism of carcinogenesis. Current researches mainly focus on energy metabolism targeted compounds, such as nucleotides, amino acids, lipids, saccharides, etc. For example, alterations of cellular lipidomics (choline, phosphatidylcholine, cholesterol, etc.) reported in cancer provides a major opportunity to treat and prevent cancer; alterations of glucose metabolism (abnormal pyruvate, lactate, and isobutyric acid, etc.) in cancer cells, which also have become the hotspots in cancer research and therapeutics by targeting lipid metabolism and glucose metabolism.
TargetMol®'s collection of 910 endogenous metabolism-related compounds, Human Endogenous Metabolite Library can be used for research in endogenous metabolism-related diseases and drug screening.

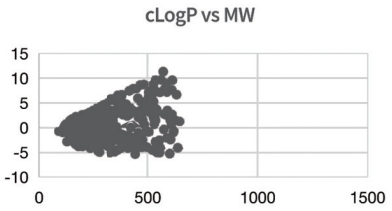
Product Advantage

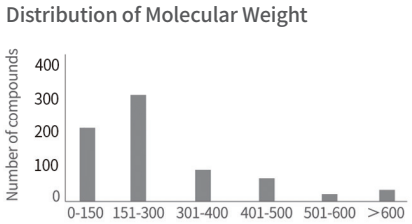
- Through searching Human Metabolome Database(HMDB)and drugBank, we collected 910 human endogenous metabolism-related compounds that are essential for normal growth and development;
- Effective tool for research in endogenous metabolism-related diseases: cancer, obesity, diabetes, etc, exploring the tumorigenesis, biomarker discovery, and drug discovery;
- Some compounds have been approved by FDA or have entered clinical trials;
- Detailed compound information with structure, activity, cell locations, biospecimen locations, tissue locations, related disese, etc.;
- NMR and HPLC/LCMS validated to ensure high purity and quality and reduce false-positive rate.

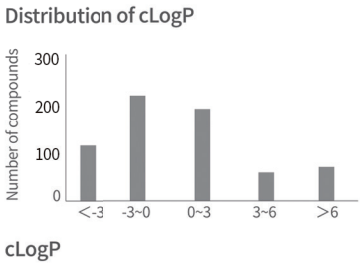
Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	13,000.00
250 µL * 10 mM (in DMSO)	USD	23,500.00
1 mg	USD	23,500.00

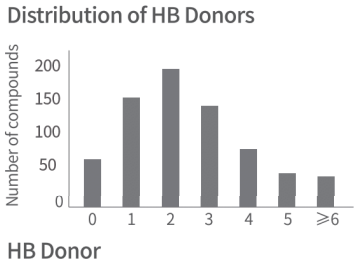
Drug-Like Properties

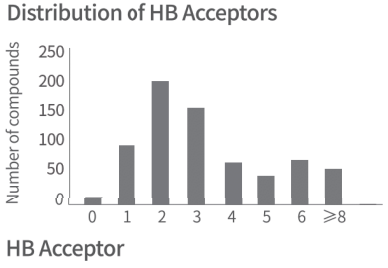
PhysChem Properties	% Compounds
<5 H-Bond donors	87
<10 H-Bond acceptors	96
cLogP<5	91
MW<500	94



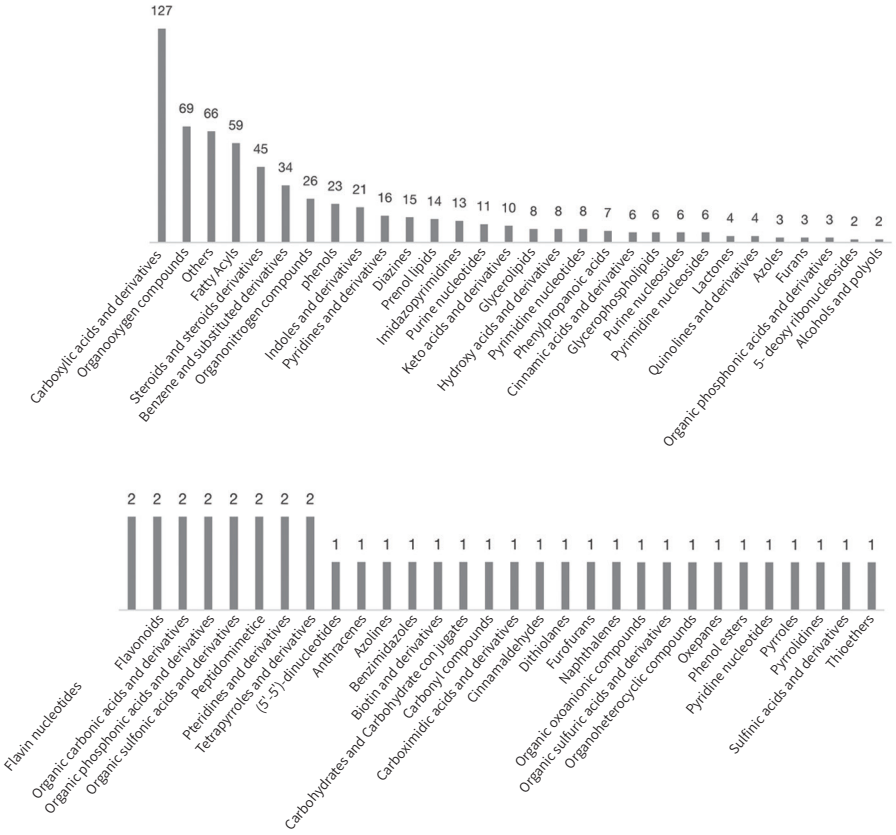




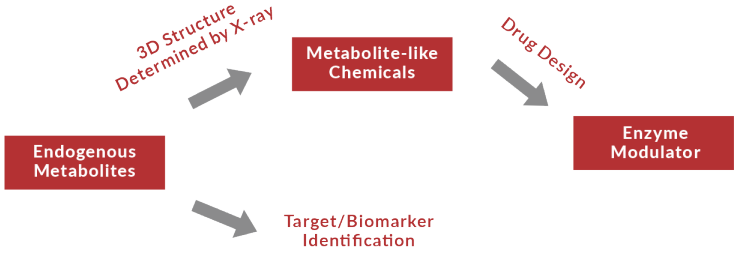




Category Composition



Why Human Endogenous Metabolite Compound Library?



Toxic Compound Library

Catalog No. L5500 — 277 compounds

TargetMol®'s Toxic Compound Library include 277 synthetic and natural toxic substances that can alter cellular, metabolic and membrane functions, such as DNA/ RNA synthesis inhibitors, cytotoxic agents, immune suppressants, anti-proliferatives, endocrine disruptors and other agents. This special collection finds application in testing the sensitivity, development and profiling of new assays in high throughput screening (HTS) programs used in new drug discovery.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	3,363.00
250 µL * 10 mM (in DMSO)	USD	5,917.00
1 mg	USD	5,917.00

Lipid Metabolism Compound Library

Catalog No. L2510 — 376 compounds

Lipids are fatty acids and their derivatives, and substances related biosynthetically or functionally to these compounds. Lipids are commonly subdivided into four main groups: fatty acids (saturated and unsaturated), glycerides (glycerol-containing lipids), nonglyceride lipids (sphingolipids, steroids, waxes), and complex lipids (lipoproteins). Like the other large biological molecules, lipids perform many different functions in a cell. Lipids are critical for cell structure, function, and energy, as well as organs and body insulation and protection. Lipid metabolism is the synthesis and degradation of lipids in cells, involving the breakdown or storage of fats for energy and the synthesis of structural and functional lipids, such as those involved in the construction of cell membranes. Lipids metabolites are extremely essential for a wide range of cellular communication and metabolism.
Numerous studies have shown that lipid metabolism plays an important role in the pathogenesis of a wide range of chronic diseases such as cardiovascular disease, aging, and cancer, etc. Lipid metabolism has now been accepted as a major metabolic pathway that is involved in many aspects of cancer cell biology. Discovering novel mechanisms of the lipid role in diseases and new ways to exploit these mechanisms for the optimal drug design would be beneficial for the prevention and treatment of these diseases.
TargetMol®'s Lipid Metabolism Compound Library collects 376 compounds acting on key targets related to lipid metabolism, such as Acetyl-CoA Carboxylase、Acyltransferase、cholesteryl ester transfer protein (CETP)、FAAH、Fatty Acid Synthase (FASN)、HMG-CoA Reductase (HMGCR), etc. It is a powerful tool that can be used in lipid metabolism-related drug development and mechanism studies.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	6,260.00
250 µL * 10 mM (in DMSO)	USD	10,281.00
1 mg	USD	10,281.00

Macrocyclic Compound Library

Catalog No. L9300 — 155 compounds

Macrocyclic compounds are highly significant in drug and research development. When developing new drugs, macrocyclic compounds are commonly researched in the medical field. Macrocyclic compounds are becoming more successfully recognized as an approach for low drug availability targets, such as antimicrobial, antiviral, and protein-protein interactions (PPIs). Topologically, macrocyclic compounds have a unique ability to span large surface areas whilst remaining conformationally restricted when compared to acyclic molecules of equivalent molecular weight. Macrocyclic compounds also reduce the overall polarity and enhance membrane permeability. Therefore, together these attributes make macrocycles a powerful approach for any lead discovery programme against challenging targets.
Research into macrocyclic compounds is increasing and is widely used in antibacterial, antiviral, and antitumor drugs for clinical applications. On antibacterial aspects, macrolides, cyclic peptides, aza-macrocyclic compounds, etc., for example, have the characteristics of broad antibacterial spectrum antibiotics. They also exhibit strong antibacterial activity, remarkable curative effect and circumvent drug resistance.
Clinical application of anti-herpes virus drugs, like ganciclovir and cidofovir have severe side effects with poor antiviral activity. Presently, attention is focused on research of naphthyridines. Some compounds already synthesized via computer technology are already exhibiting strong anti-herpes virus activity.
On anti-tumour aspects, epothilone has a similar mechanism of action as paclitaxel. Epothilone is highly toxic to cells that have developed resistance to paclitaxel, therefore overcomes the weakness displayed by paclitaxel.
With the continuous development of chemical synthesis technology, the discovery of macrocyclic lead compounds from natural products, improvement of the availability of genomic sequences and bioinformatics have marked the arrival of times of the exploration of new macrocyclic drugs. As research progresses, macrocyclic drugs are sure to have a bright application prospect.
TargetMol®'s Macrocyclic Compound Library collects 155 macrocyclic compounds of known activity for the study of macrocyclic drugs.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	4,212.00
250 µL * 10 mM (in DMSO)	USD	9,164.00
1 mg	USD	4,212.00

Mouse Metabolite Compound Library

Catalog No. L2530 — 203 compounds

TargetMol® 's Mouse Metabolite Compound Library collects 203 mouse metabolites which can be used for HTS and HCS, and research related to metabonomics.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	2,462.00
250 µL * 10 mM (in DMSO)	USD	4,331.00
1 mg	USD	4,331.00

Neural Regeneration Compound Library

Catalog No. L7700 — 149 compounds

It is well known that neurological diseases that affect the brain or other components of the central nervous system are among the most devastating and complex conditions plaguing humans today. For thousands of years, damage to the adult central nervous system (CNS) in humans has been regarded as an 'ailment which cannot be treated'. In the adult mammalian CNS, most injured axons do not regenerate, reflecting a major hurdle for functional recovery after trauma. Numerous efforts over more than a century have been devoted to uncovering the underlying mechanisms of regeneration failure. The discovery of neural and glial precursor cells in the adult brain and their ability to grow after injury trumped this assumption. However, in most cases, only small numbers of injured CNS axons can regenerate, consistent with the idea that lack of regeneration in the adult CNS is an intrinsic property of the injured neurons. Therefore, a major challenge has been to define the underlying cellular and molecular mechanisms that determine neuronal intrinsic regenerative ability, with the goal to construct a foundation for designing therapeutic neural repair strategies.
Many signaling pathways (including Ras homolog gene/Rho-associated coiled coil-forming protein kinase (Rho-ROCK), Notch, MAPK, Wnt/β-catenin, mTOR, and eph/ephrin) participate in and affect the repair or regeneration of neurons and axons in the central nervous system. The cyclic adenosine monophosphate-protein kinase A (cAMP-PKA) and Rho-ROCK signaling pathways are key signal transduction pathways for regulating neural and axonal regeneration.
TargetMol® collects 149 compounds related to neuroregeneration as Neuroregeneration Compound Library, which can be used for screening of drugs that promote axonal growth and regeneration.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	2,384.00
250 µL * 10 mM (in DMSO)	USD	4,321.00
1 mg	USD	4,321.00

Nucleotide Compound Library

Catalog No. L1720 — 203 compounds

Nucleotide analogs are nucleotides that contain a nucleic acid analogue, a sugar, and one to three phosphate groups. Nucleoside and nucleotide analogues can be used in therapeutic drugs, including a range of antiviral products used to prevent viral replication in infected cells. These agents can be used against hepatitis B virus, hepatitis C virus, herpes simplex, and HIV. Among the current antiviral drugs, almost 50% are nucleoside or nucleotide analogues. Antitumor drugs such as Cytarabine and Doxifluridine are also nucleotide analogues. The recently developed nucleoside analogues include HIV reverse transcriptase inhibitors Zidovudine, Didanosine, Zalcitabine, Stavudine, Lamivudine; Vidarabine, an antiviral drug which is active against herpes simplex and varicella zoster viruses; Acyclovir and Famciclovir, used for the treatment of herpes simplex virus infections; Ribavirin, also known as tribavirin, is an antiviral medication used to treat RSV infection, hepatitis C and some viral hemorrhagic fevers.
TargetMol®'s nucleotide compound library collects 203 nucleoside and nucleotide analogues, some of which are in the clinical trial phases or marketed therapeutic drugs, can be used for research and development of antiviral, antitumor, antifungal, and anti-depressive drugs.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	3,039.00
250 µL * 10 mM (in DMSO)	USD	5,273.00
1 mg	USD	5,273.00

Osteogenesis Compound Library

Catalog No. L7900 — 100 compounds

Bone tissue is continuously remodeled through the concerted actions of bone cells, which include bone resorption by osteoclasts and bone formation by osteoblasts. The equilibrium between bone formation and resorption is necessary and depends on the action of several local and systemic factors including hormones, cytokines, chemokines, and biomechanical stimulation. An imbalance between bone resorption and formation can result in bone diseases including osteoporosis. Osteoblasts are the main functional cells of bone formation and are responsible for the synthesis, secretion and mineralization of bone matrix. Osteoblasts undergo four stages of osteoblast proliferation, extracellular matrix maturation, extracellular matrix mineralization, and osteoblast apoptosis during bone formation. Many factors are involved in these stages to ultimately regulate bone formation.
Multiple signaling pathways were found to be involved in osteogenic proliferation and differentiation. Among them, BMP-SMAD, Wnt/β-Catenin, Notch, Hedgehog, MAPK, and FGF signaling pathways play the most critical roles in regulating osteogenic differentiation.Osteogenesis Compound Library from TargetMol® collects 100 reported osteogenesis related bioactive compounds that can be used for research in bone formation and drug screening.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	2,000.00
250 µL * 10 mM (in DMSO)	USD	3,000.00
1 mg	USD	3,000.00

Oxidation-Reduction Compound Library

Catalog No. L2900 — 453 compounds

Oxidation-Reduction Compound Library contains 453 compounds with defined prooxidant or antioxidant activity, including a variety of structurally and mechanistically different compound classes, such as hydroperoxides, polyphenolics, metal chelators, thiols, thiol traps, radical scavengers, lazaroids and glutathione modulators as well as small molecule enzyme mimetics for SOD and glutathione peroxidase. The library is a useful tool for studying the roles of pro- and antioxidant molecules in cells as well as for use in in vitro applications.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	6,925.00
250 µL * 10 mM (in DMSO)	USD	10,750.00
1 mg	USD	10,750.00

Peptide Library

Catalog No. L9600 — 440 compounds

Since Emil Fischer (Nobel Prize winner in Chemistry) published an article which reports the preparation of the first dipeptide, glycylglycine, obtained by partial hydrolysis of the diketopiperazine of glycine in the laboratory in 1901, many advances have been achieved in this field and peptides (can be defined as polypeptide chains of 50 or fewer amino acids or 5000 Da in molecular weight) have played a notable role in medical practice. In addition to Semaglutide that derived from native GLP-1 for diabetes treatment, more than 60 new synthetic peptide drugs have been approved for a wide range of conditions, cancer, infections, metabolic diseases, haematology, cardiovascular diseases, and osteoporosis.
Peptides, with size between proteins and small synthetic drugs, have crucial roles in human physiology including actions as hormones, neurotransmitters, growth factors, ion channel ligands, or anti-infectives. Peptide drugs have greater efficacy, selectivity and specificity but less toxicity.
With the advances in recombinant protein expression technologies, the development of more efficient and economic peptide synthesis, the improvement of peptide purification systems and new analytical tools, more peptide drugs have developed and entered clinical use. Smaller size and balance of conformational rigidity and flexibility have made peptides more promising candidates for drug development.
TargetMol®'s Peptide Library collects 440 peptides that can be used in peptide drug development and related mechanism study.

Pack Size		Price
1 mg	USD	4,834.00

PPI Inhibitor Library

Catalog No. L9400 — 260 compounds

Protein-protein interaction (PPI) inhibitors represent a vast class of therapeutic targets both intracellularly and extracellularly for a broad range of diseases, for instance cancer and HIV. The human interactome has been estimated to cover ~400,000 protein–protein interactions, making PPIs central to many biological processes, including enzymatic activity, assembly of protein complexes and subcellular localisation. However, PPIs are considered difficult to target. As a part of disease, biological processes are often dysregulated, therefore PPIs have become an attractive target for therapy.
TargetMol®'s PPI Inhibitor Library, a focused collection of 260 PPI-related compounds, can be used for research on protein-protein interaction.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	4,690.00
250 µL * 10 mM (in DMSO)	USD	7,800.00
1 mg	USD	7,800.00

Drug Metabolite/Impurity Library

Catalog No. L5800 — 200 compounds

Scientists have already found that the isomers or metabolites of many existing drugs show biological activity. For example, Levopropoxyphene is an antitussive, approved by FDA, but its enantiomer, Dextropropoxyphene, has an analgesic effect; L-sotalol is alpha-blocker while d-sotalol is antiarrhythmic. Currently, knowledge of isomerism has helped us in introducing safer and more effective drug alternatives of the newer as well as existing drugs. These compounds that have rich pharmacological evaluation data are ideal as entry points for drug repurposing.
The TargetMol®'s Selected drug metabolites/isomers Library, a unique collection of 200 drug isomers/metabolites with great diversity, can be used for drug screening.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	2,280.00
250 µL * 10 mM (in DMSO)	USD	3,890.00
1 mg	USD	3,890.00

Stem Cell Differentiation Compound Library

Catalog No. L8000 — 1014 compounds

Stem cells can differentiate into other types of cells and can divide to produce more of the same type of stem cells. For example, embryonic stem cells can differentiate into all the specialized cells—ectoderm, endoderm and mesoderm. Somatic stem cells are thought to be limited to differentiating into different cell types of their tissue of origin. To generate enough specialized cells or tissues that can be used for specific purposes such as tissue regeneration, cell-based therapies, drug screening, or disease models, scientists (must control the cell fate of pluripotent stem cells) are currently working on methods to effectively differentiate stem cells into functionally specialized cells. Natural and synthetic small molecules have been shown to be useful chemical tools for controlling and manipulating the fates of cells. For example, Glycogen synthase kinase 3β (GSK-3β) inhibitor could induce differentiation of neural progenitor cells (NPCs). Bone marrow stromal stem cells (BMSSCs) may have the potential to differentiate in vitro and in vivo into hepatocytes following the treatment of inhibitor of histone deacetylase and some well-defined cytokines
Stem Cell Differential Compound Library from TargetMol®, a unique collection of 1014 stem cell differentiation signaling targeted compounds, can be used for stem cell research and related drug screening (high throughput and high content screening).

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	16,876.00
250 µL * 10 mM (in DMSO)	USD	27,711.00
1 mg	USD	27,711.00

Target-Focused Phenotypic Screening Library

Catalog No. L9500 — 1832 compounds

TargetMol® offers a high-quality Target-focused Phenotypic Screening Library (1832 compounds in total) with maximal biological and chemical diversity for such empirical approaches. Phenotypic approaches use semi-empirical methods that do not require much knowledge of the target and understanding of the mechanism. A recent analysis revealed the phenotypic approaches to be the more successful strategy for small-molecule, first-in-class medicines. The rationalization for this success was the unbiased identification of the molecular mechanism of action (MMOA). In addition, an understanding of mechanism is not required for regulatory approval; the regulatory agencies are less concerned with the MMOA of a compound than with whether it is effective. It can be argued that in seeking the best path to new medicines, academic science should be focusing not on gene-based, hypothesis-driven research but on translating disease knowledge into disease-relevant phenotypic assays for screening and chemical biology approaches to screening and target identification as well as on systematic approaches to understanding the MMOA. Greater focus on translational research should lead to greater access to more reliable phenotypic assays.
The use of well-annotated bioactive compounds with clear targets for phenotypic screening can also narrow the scope of targets that are needed to be validated, therefore, it is an effective tool for target identification or validation.
Given the potential applications of a Phenotypic Screening Library, the focus of the compounds selection strategy lies on biodiversity and maximal coverage of chemical space, aimed at providing hits for a wide spectrum of biological goals. This library was finally developed to contain a set of compounds with confirmed biological activity for more than 600 drug targets and includes 2-4 structurally diverse compounds for each target.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	14,280.00
250 µL * 10 mM (in DMSO)	USD	23,800.00
1 mg	USD	23,800.00

Transcription Factor-Targeted Compound Library

Catalog No. L1380 — 449 compounds

Transcription factor (TF) (or sequence-specific DNA-binding factor) is a protein that controls the rate of transcription of genetic information from DNA to messenger RNA, by binding to a specific DNA sequence. The function of TFs is to regulate—turn on and off—genes in order to make sure that they are expressed in the right cell at the right time and in the right amount throughout the life of the cell and the organism. TFs function in a coordinated fashion to direct cell division, cell growth, and cell death throughout life; cell migration and organization (body plan) during embryonic development; and intermittently in response to signals from outside the cell, such as a hormone. There are up to 2600 TFs in the human genome.
TargetMol®'s Transcription Factor-Targeted Compound Librarycollects 449 compounds with unique structures targeting 13 different transcription factors with IC50 value below 2.5 µM, is a supplemental tool for research in cell division and cell cycle regulation.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	4,690.00
250 µL * 10 mM (in DMSO)	USD	7,800.00
1 mg	USD	7,800.00

Natural Product Library for HTS

Natural Product Library for HTS

Catalog No. L6000 — 2960 compounds

Product Description

Natural products are an unsurpassed source of chemical diversity and an ideal starting point for any screening program for pharmacologically active small molecules. Historically, natural products have been the most successful source of new drugs. From 1981 to date, 79 (80%) out of 99 small molecule anticancer drugs are natural product-based/inspired, with 53 (53%) being either natural products or derived therefrom. Natural products have been proven to be successful modulators of difficult targets such as a range of antibacterial targets and, especially, protein–protein interactions. Furthermore, many researchers consider natural products and their derivatives as privileged tools for the study and manipulation of protein function.
The TargetMol®'s Natural Product Monomers (HTS) Library, a unique collection of 2960 natural products with known bioactivity, wide source, and cost-effectiveness, is a powerful tool for drug discovery, pharmacological study, stem cell differentiation, fingerprint study and quality research, etc.

Product Advantage

- A unique collection of 2960 pure natural products and their derivatives with known biological activity for drug discovery;
- Structurally diverse: 2960 natural products including more than 30 types of chemicals, such as alkaloids, limonoids, sequiterpenes, diterpenes, pentacyclic triterpenes, sterols, and many other diverse representatives;
- Documentation with clear source: isolated natural products from plant, animal, and microorganism. Detailed compound information with structure, solubility, target, activity, and biological activity description;
- Cost-effective to save your fundings;
- Can be highly customized: specific compounds, quantities, format (dry/solid or DMSO), plate map, and concentration to meet your specific requirement.

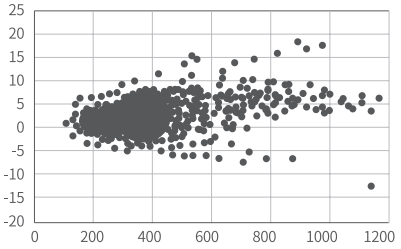
Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	29,240.00
250 µL * 10 mM (in DMSO)	USD	48,374.00
1 mg	USD	48,374.00

Drug-Like Properties

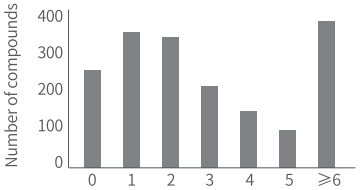
% of compounds compliant with Lipinski' s Rules

PhysChem Properties	% Compounds
<5 H-Bond donors	73
<10 H-Bond acceptors	80
cLogP<5	91
MW<500	79

cLogP vs MW

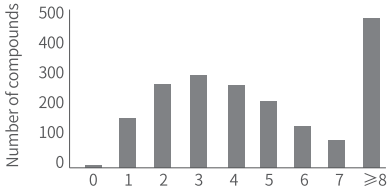


Distribution of HB Donors



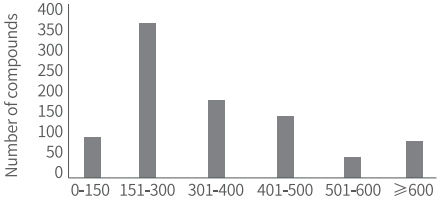
HB Donor

Distribution of HB Acceptors



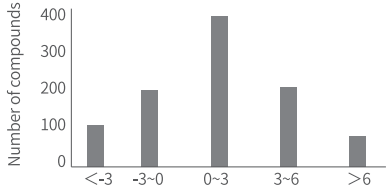
HB Acceptor

Distribution of Molecular Weight



Molecular Weight

Distribution of cLogP



cLogP

Compound Library	Size	Comments
Selected Plant-Sourced Compound Library L4600	1990	A unique collection of 1990 plant-sourced compounds that derived from 277 plant species; Detailed information: structure, solubility, target, activity, and biological activity description; Structurally diverse, medicinally active, and cell permeable; Includes many popular natural products, such as Artemisinin, Ginsenoside, etc.
Polyphenolic Natural Product Library L6100	411	Polyphenols are compounds with various potential biological properties such as antioxidants, anti-inflam matory, antineoplastic, antiaging, cardioprotective, anticancer, and antimicrobial properties; Natural polyphenols include flavonoids, phenolic acids, lignans, tannins, stilbenes, curcumin, coumarin, quinone, and other polyphenols; Structurally diverse, medicinally active, and cell permeable.
Chinese Pharmacopoeia Natural Product Library L6800	1339	1339 natural products carefully selected from Chinese Pharmacopoeia (CP) Dictionary, including active ingredients from 246 traditional Chinese herb medicine, such as Danshen (Salvia miltiorrhiza), Eucommia ulmoides, Huangqi (Astragalus), etc; Diversified structures: including flavonoids, polyphenols, Alkaloids, etc. ; Clear source: known active natural products selected from animals, plants, or microorganisms with clear species information.
Selectable Natural Product Library L6020	17580	17580 pure natural products with diverse structures and sources covering various plant, animal, and microbe species; Free SDF data available for each compound structure in this library, an effective tool for virtual screening; All products can be resupplied.
Anti-Tumor Natural Product Library L6700	1059	Known bioactivity for all compounds: detailed biological and pharmacological information, providing the research foundation and theoretical direction for screening; Clear source: known active natural products selected from animals, plants, or microorganisms with clear species information; Cost-effectiveness: expensive natural products with poor drug likeliness are excluded, allowing for more high-quality natural products at a lower cost.

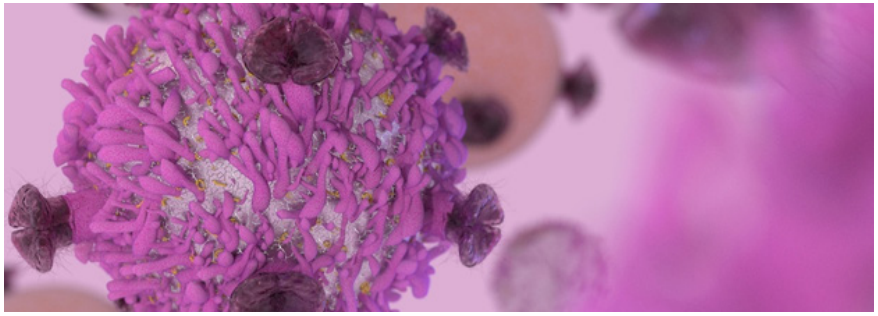
Characteristic Natural Product Libraries

Alkaloid Natural Product Library

Catalog No. L6110 — 317 compounds

Alkaloids are a class of naturally occurring organic compounds that mostly contain basic nitrogen atoms, and are mainly produced by plants. A large amount of research has found that alkaloids have a wide range of pharmacological activities including antimalarial (e.g. quinine), antiasthma (e.g. ephedrine), anticancer (e.g. homoharringtonine), cholinomimetic (e.g. galantamine), vasodilatory (e.g. vincamine), antiarrhythmic (e.g. quinidine), analgesic (e.g. morphine), antibacterial (e.g. chelerythrine), and antihyperglycemic activities (e.g. piperine). Many have found use in traditional or modern medicine, or as starting points for drug discovery. As research in alkaloids advances, alkaloids would play an important and visible role in modern drug development and provide a continuing source of novel drug leads.
TargetMol®'s Alkaloid Natural Product Library carefully collects 317 alkaloids derived from plants, including Aconite, Periwinkle, Camptotheca acuminate, Belladonna, Coptis chinensis, etc. They have anticancer, anti-inflammatory, anti-oxidative, and neuroprotective effects. For example, vinca alkaloids obtained from Madagascar periwinkle plant are important for being cancer fighters and are the second-most-used class of cancer drugs and will stay among the original cancer therapies. Lycorine, one of the main alkaloids of the Amaryllidaceae family, was found to be responsible for the pronounced antiviral and antibacterial activity of the crude extracts from the roots and leaves of Clivia miniata Regel. Tetrahydropalmatine, an isoquinoline alkaloid that is considered the active ingredient of Corydalis yanhusuo, has significant analgesic effects.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	5,700.00
250 µL * 10 mM (in DMSO)	USD	9,510.00
1 mg	USD	9,510.00



Anti-COVID-19 Traditional Chinese Medicine Compound Library

Catalog No. L6720 — 486 compounds

During the treatment of Covid-19 in China, the intervention of traditional Chinese medicine (TCM) reduced the severe symptoms of patients and played a significant role in the war against COVID-19. Multiple research studies indicated TCM exerted an overall regulatory effect via multi-component and multi-target network. TCM could suppress endotoxin-induced cytotoxicity, kill the virus, reduce the virus' access to the cell and lower the incidence of a cytokine storm. To further support the research in modes of action of TCM in the treatment of COVID-19, we extracted 486 bioactive components (monomers) from TCM prescriptions having therapeutic effects.
This library collects monomers of diverse structures, such as Flavonoids, alkaloids, Polyphenols, Terpenes, ets., from TCM prescriptions of significant therapeutic effect on COVID-19 including Lonicera japonica Thunb., Forsythia suspensa, Scutellaria baicalensis Georgi, Bupleuri Radix, Agastache rugosa, Isatidis Radix, Rhodiola rosea, etc.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	8,778.00
250 µL * 10 mM (in DMSO)	USD	14,630.00
1 mg	USD	14,630.00

Anti-Inflammatory Traditional Chinese Medicine Compound Library

Catalog No. L6710 — 319 compounds

Inflammation is part of the complex biological response of body tissues to harmful stimuli, such as pathogens, damaged cells, or irritants, and is a protective response involving immune cells, blood vessels, and molecular mediators. The classical characteristics of inflammation are pain, swelling, edema, redness and heat. Anti-inflammatory drugs are the second most commonly clinically used drugs. The widely used anti-inflammatory drugs include nonsteroidal anti-inflammatory drugs (NSAIDs) and corticosteroids. However, both have a wide range of side effects. As research advanced, various natural products from traditional Chinese medicine (TCM) have been demonstrated in many animal or cell culture models to safely suppress proinflammatory pathways and control inflammation-associated disease. Plant chemical constituents are one of the richest hot spots for the most significant new drug discoveries. Herbal medicines have gained special interest in recent years as a subject of both commercial and scientific interests.
TargetMol® collects 319 TCM monomers with anti-inflammatory activity in this library, including Flavone, Saponins, Terpenes, Alkaloids, etc. derived from herbs such as honeysuckle, Coptis chinensis, Baical Skullcap Root, Panax notoginseng, etc. With its diversity of compound structures and detailed information about bioactivity, it is a powerful tool for research in anti-inflammation.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	5,742.00
250 µL * 10 mM (in DMSO)	USD	9,570.00
1 mg	USD	9,570.00

Anti-Tumor Natural Product Library

Catalog No. L6700 — 1059 compounds

Cancer is a well-recognized global health problem responsible for 7.6 million deaths (13% of all deaths) worldwide, which is expected to rise to 13.1 million by 2030. It has long been recognized that natural products represent the richest source of high chemical diversity, providing the basis for identification of novel scaffold structures that serves as starting points for rational anticancer drug design. According to a recent review, 49% of drugs were either natural products or their derivatives that are used in cancer treatment. Moreover, between the years 2005 and 2010, 19 natural product-based drugs have been approved, among which 7, 10 and 2 have been classified as natural product (NP), semi-synthetic NPs and NP-derived drugs, respectively. Natural products have served as an effective source of drugs and drug leads. TargetMol® carefully collects 1059 natural products from plants, animals, or microbes with known or potential antitumor activity, which is a powerful tool for your antitumor drug development and lead compounds screening.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	17,222.00
250 µL * 10 mM (in DMSO)	USD	28,830.00
1 mg	USD	28,830.00

Flavonoid Natural Product Library

Catalog No. L6120 — 252 compounds

Flavonoids (or bioflavonoids) are a class of plant and fungus secondary metabolites. Chemically, flavonoids have the general structure of a 15-carbon skeleton, which consists of two phenyl rings (A and B) and a heterocyclic ring (C). This carbon structure can be abbreviated C6-C3-C6. Its backbone is 2-phenyl-1,4-benzopyrone. Flavonoids are served as the major active ingredients in traditional Chinese herbal medicines. Several lines of evidence support that flavonoids have impacts on many aspects of human health, including antitumor, anti-oxidative, antibacterial, anti-inflammation, and cardiovascular protective effects. The mechanism of action involves scavenging free radicals, down-regulating several inflammatory mediators, inhibiting energy metabolism, stimulating enzymatic activity of DNA-dependent RNA polymerase 1 and subsequent biosynthesis of RNA and protein, inhibiting biosynthesis of protein cytokines, and regulating cell cycle, etc.
TargetMol®'s Flavonoid Natural Product Library collects 252 flavonoids derived from much traditional Chinese medicine such as Ginkgo, Radix Sophorae Flavescentis, Radix Astragali, Lonicera japonica, Epimedii Folium, etc. Compounds in the library involve multiple physiological functions, such as Rutin and Quercetin have anti-inflammatory, analgesic, antioxidant, and decreasing blood pressure effects; Hesperidin has antioxidant and anti-inflammatory properties; Luteolin, Baicalein, and Baicalin all have antibacterial effects; Genistein has been identified as angiogenesis inhibitors, and found to inhibit the uncontrolled cell growth of cancer.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	4,536.00
250 µL * 10 mM (in DMSO)	USD	7,560.00
1 mg	USD	7,560.00

Food as Medicine Compound Library

Catalog No. L6300 — 588 compounds

Hippocrates was to thank for the famous quote, "Let food be thy medicine and medicine be thy food". Hippocrates and the Ancient Greeks weren't the only ones onto something when they studied the many medicinal properties of foods. Many traditional systems of healing which have been practiced throughout history — including Ayurvedic Medicine and Traditional Chinese Medicine, for example — have taught for thousands of years that food is medicine and a healthy diet is a powerful tool for protecting one's health. In 2014, The National Health and Family Planning Commission (NHFPC) of China released the draft "Administrative Measures on the Catalogue of Substances Traditionally Considered as Both Food and Chinese Medicine" for public consultation. There are 101 substances included in the Catalogue.
Based on the food as medicine raw materials published by NHFPC and related literature, TargetMol® carefully collects 588 compounds with safety guaranteed as Food as Medicine Compound Library, which can be used for high throughput and high content screening for drug discovery.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	9,790.00
250 µL * 10 mM (in DMSO)	USD	16,070.00
1 mg	USD	16,070.00

Microbial Natural Product Library

Catalog No. L6500 — 134 compounds

Microscopic organisms, commonly known as microorganisms or microbes, are found all around us and even inside our bodies, including a massive range of organisms including bacteria, fungi, viruses, algae, archaea and protozoa. The vast majority of microbes on the earth pose no real threat to humans, plants or animals; in fact they actually work alongside humans to make the world go round, aiding decomposition, decay and even helping us to digest our food. Microorganisms are renowned as a prolific source of natural products, making huge contributions to human health. The 1945 and 1952 Nobel Prizes in Physiology or Medicine were awarded for the discovery of penicillin and streptomycin, respectively. Six years later, the 2015 Nobel Prize in Physiology or Medicine was awarded to William C. Campbell and Satoshi Omura, and Youyou Tu for the discovery of avermectins and artemisinin, respectively, therapies that revolutionized the treatment of devastating parasite diseases. Among these four natural products awarded with Nobel Prizes, except for artemisinin, the other three are all microbial natural products. Streptomyces is the important source for natural medicines, the largest antibiotic-producing genus, producing antibacterial (vancomycin and daptomycin, etc.), antifungal (nystatin, amphotericin B, and natamycin), and antiparasitic drugs (Ivermectin), and also a wide range of other bioactive compounds used in other medical treatment, such as anticancer drugs (dactinomycin and bleomycin).
Microbial Natural Product Library is a unique collection of 134 microbial natural products covering various chemical structures, such as β-lactam, macrolides, aminoglycoside, polypeptides, Chloramphenicol, Tetracycline compounds, Anthraquinone, Benzene derivatives, quinone, Terpenoids, etc. This library can be used in rational drug design, virtual screening, and microbes classification, etc.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	2,152.00
250 µL * 10 mM (in DMSO)	USD	3,891.00
1 mg	USD	3,891.00

Chinese Pharmacopoeia Natural Product Library

Catalog No. L6800 — 1339 compounds

Traditional Chinese medicine has been practiced for thousands of years, and is now receiving rigorous research thanks to the isolation of active ingredients and a better understanding of mechanisms of action. For example, Artemisinin, the active ingredient extracted from a Chinese materia medica Artemisia annua, is the most effective antimalarial drug. Ginsenosides are a class of natural product steroid glycosides and triterpene saponins. Compounds in this family are found almost exclusively in the plant genus Panax (ginseng), which has a long history of use in traditional medicine. Therefore, it is a good and economical way to discover new chemical drugs based on active ingredients and leading compounds separating from Chinese herbal medicine and it may be an available path with less risk. With the continuous development of the traditional Chinese medicine industry in recent years, it is proved that traditional Chinese medicine (TCM) monomers have a marked effect for treating some diseases.
Chinese Pharmacopoeia Natural Product Library by TargetMol® consists of 1339 natural products carefully selected from Chinese Pharmacopoeia (CP) Dictionary, including 246 active ingredients from traditional Chinese herb medicine, such as Danshen (Salvia miltiorrhiza), Eucommia ulmoides, Huangqi (Astragalus), etc. which is a powerful tool for research in antitumor, antibacterial, apoptosis, and autophagy. These Chinese medicine monomers consist of greatly diversified structures, such as Genistein, polyphenols, β-Carotene, Ursolic acid, Flavonoids, and Saponins, etc. with known bioactivity information that will assist you in improving the drug screening success rate.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	22,300.00
250 µL * 10 mM (in DMSO)	USD	36,500.00
1 mg	USD	36,500.00

Polyphenolic Natural Product Library

Catalog No. L6100 — 411 compounds

Polyphenols are compounds with various potential biological properties such as antioxidants, anti-inflammatory, antineoplastic, antiaging, cardioprotective, anticancer, and antimicrobial properties. Natural polyphenols play an important role in cancer prevention and treatment by blocking cell cycle, inducing apoptosis, and inhibiting cell adhesion, migration, proliferation, and differentiation. Polyphenols are defined as compounds having at least one aromatic ring with one or more hydroxyl functional groups attached. Natural polyphenols include flavonoids, phenolic acids, lignans, tannins, stilbenes, curcumin, Coumarin, quinone, and other polyphenols.
Polyphenolic Natural Product Library is a unique collection of 411 natural polyphenolic compounds, an effective tool for anticancer drug screening and high throughput screening (HTS) and high content screening (HCS).

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	7,458.00
250 µL * 10 mM (in DMSO)	USD	12,279.00
1 mg	USD	12,279.00

Rare Natural Product Library

Catalog No. L6900 — 284 compounds

Natural products are an unsurpassed source of chemical diversity and an ideal starting point for any screening program for pharmacologically active small molecules. Historically, natural products have been the most successful source of new drugs. From 1981 to date, 79 (80%) out of 99 small molecule anticancer drugs are natural product-based/inspired, with 53 (53%) being either natural products or derived therefrom. Natural products have been proven to be successful modulators of difficult targets such as a range of antibacterial targets and, especially, protein–protein interactions. Furthermore, many researchers consider natural products and their derivatives as privileged tools for the study and manipulation of protein function.
The TargetMol®'s Rare Natural Product Library, a unique collection of 284 rare natural products with known bioactivity and wide source, is a powerful tool for drug discovery, pharmacological study, and stem cell differentiation, etc.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	4,188.00
250 µL * 10 mM (in DMSO)	USD	6,895.00

Saccharide and Glycoside Natural Product Library

Catalog No. L6140 — 364 compounds

Saccharides is a general term for polyhydroxy (two or more) aldehyde or ketone compounds, and their derivatives or polymers, including sugars, starch, and cellulose, are widely distributed in nature. Saccharides and their derivatives play key roles in the immune system, fertilization, preventing pathogenesis, blood clotting, and development, such as Lentinan, a polysaccharide derived from the vegetative parts of the edible Japanese shiitake mushroom, boosting humoral antitumor immunity; Astragalus polysaccharide (APS) enhances the immune organ index, promotes the proliferation of immune cells, stimulates the release of cytokines, and affects the secretion of immunoglobulin and conduction of immune signals.
Glycosides are a wide variety of naturally occurring substances in which a sugar group is bonded through its anomeric carbon to another group of a non-sugar via a glycosidic bond. Many glycosides occur in plants, often as flower and fruit pigments; for example, anthocyanins. Glycosides play numerous important roles in living organisms, such as Gastrodin exhibits a neuroprotective effect (used in the treatment of dizziness, paralysis, epilepsy, stroke and dementia); Notoginsenoside exhibits anti-inflammatory, anti-oxidative and anti-apoptotic properties.; cardiac glycoside is used in the treatment of mild to moderate heart failure and for ventricular response rate control in chronic atrial fibrillation; Flavonoid glycosides exhibit anti-inflammatory, relieving cough and asthma, and dilating coronary artery effects, etc.
TargetMol®'s Saccharide and Glycoside Natural Product Library collects 364 saccharides and glycosides, such as Ginsenosides, Neohesperidin, Saikosaponin, Salidroside, Notoginsenoside, cardiac glycoside, Flavonoid glycosides, etc.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	6,547.00
250 µL * 10 mM (in DMSO)	USD	10,920 .00
1 mg	USD	10,920 .00

Selected Plant-Sourced Compound Library

Catalog No. L4600 — 1990 compounds

Nature, the master of craftsman of molecules created almost an inexhaustible array of molecular entities. It stands as an infinite resource for drug development, novel chemotypes and pharmacophores, and scaffolds for amplification into efficacious drugs for a multitude of disease indications and other valuable bioactive agents. Plants have been the basis of many traditional medicine systems throughout the world for thousands of years and continue to provide humans with new remedies. The use of plants as medicines has a long history in the treatment of various diseases. The plant-derived compounds have a long history of clinical use, better patient tolerance and acceptance. To date, 35,000-70,000 plant species have been screened for their medicinal use. The first commercial pure natural product introduced for therapeutic use is morphine marketed by Merck in 1826, and the first semi-synthetic pure drug aspirin, based on a natural product salicin isolated from Salix alba, was introduced by Bayer in 1899. This led to the isolation of early drugs such as cocaine, codeine, digitoxin, quinine and pilocarpine, of which some are still in use and several other recent plant-derived compounds, which have undergone development and have been marketed as drugs which include Paclitaxel from Taxus brevifolia for lung, ovarian and breast cancer, Artemisinin from traditional Chinese plant Artemisia annua to combat multidrug resistant malaria, Silymarin extracted from the seeds of Silybum marianum for the treatment of liver diseases.
The TargetMol®'s Selected Plant-Sourced Compound Library, a unique collection of 1990 plant-sourced compounds that derived from 277 plant species, can be used for natural drug screening and new drug development.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	24,493.00
250 µL * 10 mM (in DMSO)	USD	34,399.00
1 mg	USD	34,399.00

Terpene Natural Product Library

Catalog No. L6130 — 349 compounds

Terpenes are a large and diverse class of organic compounds, produced by a variety of plants, particularly conifers, and by some insects. They are also called isoprenoids—are made up of isoprene molecules. The building block is a five-carbon isoprene (CH2C(CH3)CHCH2) unit. Herbs and higher plants containing their oxidized derivatives, known as terpenoids, have been used for centuries as flavors, fragrances and pharmaceuticals. More than 22000 terpenoids are known at present, which makes this the largest group of natural compounds. Studies in recent decades have demonstrated that terpenes exert anti-inflammatory, anticancer, antimalaria, decreasing blood pressure effects. Screening against terpene compound library would provide research basis for the application of terpenoids.
TargetMol®'s Terpene Natural Product Library collects 349 terpenoids including mono-, sesqui-, di-, and triterpenes, corresponding to 10, 15, 20 and 30 carbon atoms, covering research areas such as cancer, immunology, inflammation, metabolism, etc.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	8,196.00
250 µL * 10 mM (in DMSO)	USD	13,667.00
1 mg	USD	13,667.00

Traditional Chinese Medicine Monomer Library

Catalog No. L6810 — 2104 compounds

Traditional Chinese medicine has been practiced for thousands of years to treat or prevent diseases. However, its physical foundation, mode of action, and prescription compatibility of TCM pharmacodynamic action were not determined in complete detail, and the complexity of formulae greatly limited the research of effective constituents related to the clinical efficacy of TCM. The therapeutic efficacy of TCMs is mainly based on the combined action of a mixture of active phytochemical constituents. Nearly 200 modern medicines have been developed either directly or indirectly from the plants used as medicines in China. For example, Artemisinin, the active ingredient extracted from a Chinese herb Artemisia annua L, is the most effective antimalarial drug. Ginsenosides are a class of natural product steroid glycosides and triterpene saponins. Compounds in this family are found almost exclusively in the plant genus Panax (ginseng), which has a long history of use in traditional medicine. Therefore, it is a good and economical way with less risk to discover new chemical drugs based on active ingredients and leading compounds separating from Chinese herbal medicine. With the continuous development of the traditional Chinese medicine industry especially in separation methods and isolation techniques in recent years, it has been proved that traditional Chinese medicine (TCM) monomers, the active compounds of Chinese Herbal Medicines, have many medicinal properties and can effectively guide innovative drug discovery.
TCM can contribute to addressing a number of global health challenges of the 21st Century, in particular in the area of chronic, noncommunicable diseases and population aging.
TargetMol®'s Traditional Chinese Medicine Monomer Library collects 2104 compounds that all come from about 300 Chinese Herbal Medicines, such as Panax natoginseng, Licorice, Angelica, Pericarpium Citri Reticulatae, Coptis chinensis, Panax ginseng, etc., containing chemical structures such as Flavonoids, Alkaloids, Terpenes, Glycosides, etc. TargetMol®'s Traditional Chinese Medicine Monomer Library is a useful tool for new drug discovery and mechanism studies in anticancer, anti-inflammatory, antibacterial, apoptosis, autophagy, etc.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	27,709.00
250 µL * 10 mM (in DMSO)	USD	43,874.00
1 mg	USD	43,874.00

Tibetan Medicine Compound Library

Catalog No. L6210 — 239 compounds

Tibetan medicine is a unique system of medicine formed through long-term practice on the basis of extensive absorption and integration from Chinese medicine, Indian medicine and Arabic medicine, with a history of thousands of years. It is one of the relatively complete and influential national medicines in China.
The vast territory of the Tibetan Plateau and the complex dynamic natural conditions have contribute d to its diverse flora and fauna resources.
Historically, the Tibetan region is a large treasure trove of Chinese medicinal plants. According to preliminary statistics, more than a thousand kinds of wild medicinal plant resources can be found in the Tibetan region. For instance, Cordyceps (Dong Chong Xia Cao), Fritillariae Cirrhosae Bulbus (Chuan Bei Mu), notoginseng (Tian Qi), Gastrodiae Rhizoma (Tian Ma), Ganoderma lucidum (Ling Zhi) are valuable medicinal materials that sells worldwide; Cephalotaxus hainanensis (Hai Nan Cu Fei), Taxus Chinensis (Hong Dou Shan), Dysosma versipallis rhizome (Gui Jiu), Dysosma versipellis (Ba Jiao Lian), Arnebia euchroma (Ruan Zi Cao), Sageretia Gracilis (Xian Xi Que Mei Teng), Lilium brownie (Ye Bai He) are plants with development potential; and the Library includes other common traditional mecinal herbs like Amomum Villosum (Sha Ren), Uncaria Rhynchophylla (Gou Teng), Gentiana Macrophylla (Qin Jiao), Tree Peony Bark (Dan Pi), Papaya, Rhizoma Paridis (Zhong Lou), Ephedra (Ma Huang), Semen Persicae (Tao Ren), Coptis (Huang Lian), Bupleurum (Chai Hu), Chinese Angelica Root (Dang Gui), Astragalus (Huang Qi), Gentiana scabra (Long Dan), Codonopsis pilosula (Dang Shen), Aconitum (Wu Tou), Rhubarb (Da Huang), Barberry Root (San Gen Zhen), Snow Lotus Herb (Xue Lian Hua), Schisandra Chinensis (Wu Wei Zi) etc.
Tibetan medicine has a long history of profound sophistication. In order to facilitate researchers to study the mechanism of action of active ingredients in Tibetan medicine and conduct related drug development, we have collected a total of 239 natural product molecules derived from dozens of Tibetan medicines. The sources include Cordyceps, Rhodiola, Saffron, Tianshan Snow Lotus, Ganoderma and other precious herbs, which can be used for high-throughput and high-content screening.

Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	4,319.00
250 µL * 10 mM (in DMSO)	USD	7,195.00
1 mg	USD	7,195.00

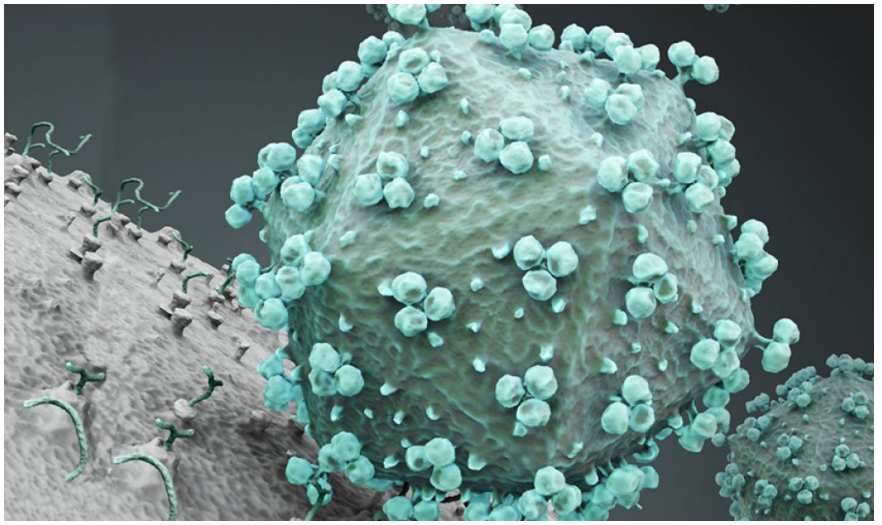
Natural Product Derivatives Library

Natural Product Derivatives Library

Catalog No. NY1000 — 4000 compounds

Historically, natural products have been pharma's treasure trove. According to the Natural Product Derivatives Library Initiative at the Scripps Research Institute, "from the 1940s to date, 131 (74.8%) out of 175 small molecule anticancer drugs are natural product-based/inspired, with 85 (48.6%) being either natural products or derived therefrom. From 1981 to date, 79 (80%) out of 99 small molecule anticancer drugs are natural product-based/inspired, with 53 (53%) being either natural products or derived therefrom. “In a sense, this is not surprising. In nature, after all, creatures — and at the more basic level, structures, such as receptors and their ligands — have been co—evolving for billions of years.

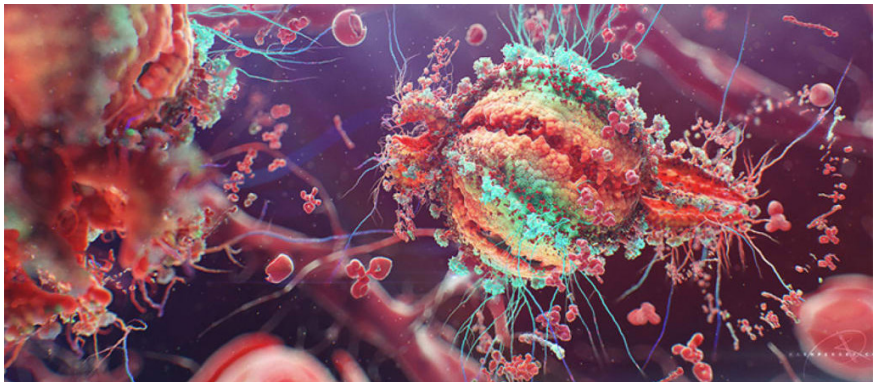
Pack Size		Price
100 µL * 10 mM (in DMSO)	USD	35,058.00



Selectable Natural Product Library

Catalog No. L6020 — 17580 compounds

Nature is a rich source of producing natural products by biosynthetic enzymes in a living organism, and most of which are structurally unique and difficult to be man-made synthesized. From 1981 to date, 79 (80%) out of 99 small molecule anticancer drugs are natural product-based/inspired, with 53 (53%) being either natural products or derived therefrom. Nature represents a major source of innovative therapeutic agents, and natural products still are recognized as an indispensable source for drug discovery. The 2015 Nobel Prize awarded to Professor Youyou Tu was to recognize and appreciate her pioneering discovery of artemisinin fromArtemisia annuaand clinical innovation in fighting against malaria, one of the top three diseases leading to the loss of people’ s life.This award not only recognizes their achievements but spotlights the rich resource of natural products that show promise in medicine andhealth, attracting the interest of more scientists in the natural product discovery.
Currently screening hits from anatural product library then structurally optimizing hits to new drugs with therapeutic effects is an important way to the development of new drugs. Many natural product databases can provide data on structures concerning hundreds of thousands of natural product monomers, but most of which are not physically exist to be acquired.
In this library, TargetMol® carefully select 17580 diverse natural products with free SDF data available to facilitate your research and development. It is a powerful tool for virtual screening, new drug development, and pharmacological study.



Featured Fragment Library

Catalog No. L5700 — 246 compounds

Fragment-based drug discovery (FBDD) has emerged in the past decade as a powerful tool for discovering drug leads. FBDD has played a role in the discovery of at least 30 drugs that are in various stages of clinical development, and practitioners of FBDD can be found throughout the world in both academia and industry. Different from HTS, FBDD finds fragment-like hits (molecular weight less than 300) that usually bind with low affinity; therefore, sensitive detection methods are required, such as sensitive biophysical techniques: X-ray crystallography, NMR, Surface Plasmon Resonance (SPR), or mass spectrometry. This strategy offers several attractive features compared with traditional HTS or virtual screening, including higher hit rate, higher binding efficiency, and providing multiple starting points for further structural optimizations. In addition, because of the exponentially growing amount of information about one certain target, the effective utilization of bioinformatics and chemoinformatics is expected to contribute markedly toward the discovery of new drugs.
The TargetMol®'s Fragment Library collects 246 fragment-like small molecules for drug discovery.

Pack Size		Price
1 mg	USD	3,080.00
5 mg	USD	5,655.00
10 mg	USD	9,057.00

High Solubility Fragment Library

High Solubility 3D Diversity Fragment Library

Catalog No. L7850 — 1083 compounds

The highly soluble structural diversity fragment compound library is constructed in an efficient and modular manner, so it is very suitable for solving the current situation that a large amount of synthetic investment is required to achieve multi-directional fragment growth. The structurally diverse fragments are designed to contain suitable synthetic reactive groups for future fragment growth. The library of highly soluble 3D structural diversity fragments contains 1083 compounds.

Pack Size		Price
1 mg	USD	11,312.00
5 mg	USD	26,565.00
10 mg	USD	35,763.00

High Solubility Fragment Library

Catalog No. L7800 — 2746 compounds

The TargetMol®'s Fragment Library Plus collects 2746 fragment-like small molecules meeting with strict Astex Rule of Three Criteria (MW ⩽ 300, cLogP ⩽ 3, H-bond donors ⩽ 3 H-bond acceptors ⩽ 3) for fragment-based drug discovery.

Pack Size		Price
1 mg	USD	24,941.00
5 mg	USD	58,573.00
10 mg	USD	78,853.00

High Solubility FragLite Fragment Library

Catalog No. L7840 — 796 compounds

The High Solubility FragLite Fragment Library contains small halogenated fragments and halogenated peptide mimic fragments. FragLites are small halogenated fragments that can be used to effectively map drug interactions in new proteins. PepLites is a small halogenated peptide mimic, designed in parallel with FragLites to cover a wider range of drug interactions in new proteins. The highly soluble halogenated fragment library contains 796 halogenated fragment compounds.

Pack Size		Price
1 mg	USD	9,037.00
5 mg	USD	21,223.00
10 mg	USD	28,572.00

High Solubility Micro Fragment Library

Catalog No. L7820 — 1082 compounds

The compound library of highly soluble micro-fragments consists of 1082 low-molecular-weight fragments. Low-molecular-weight compounds (so-called micro-fragments) are derived from commercially available fragment spaces. The focus is on ensuring the chemical stability of the compound, the absence of reactive compounds, meeting the physical and chemical characteristics of the screening, and not strictly complying with the drug similarity standards, the structural diversity of compounds/covering a wider chemical space, aims to provide hit drug targets for the fields of new drug discovery and drug design.

Pack Size		Price
1 mg	USD	11,301.00
5 mg	USD	26,541.00
10 mg	USD	35,730.00

High Solubility Pharmacophore Fragment library

Catalog No. L7830 — 985 compounds

Fragment-based drug design has introduced a bottom-up process for drug development, with improved sampling of chemical space and increased effectiveness in early drug discovery. Here, we combine the use of pharmacophores, the most general concept of representing drug-target interactions with the theory of protein hotspots, to develop a design protocol for fragment libraries. The SpotXplorer approach compiles small fragment libraries that maximize the coverage of experimentally confirmed binding pharmacophores at the most preferred hotspots. Our carefully selected High Solubility Pharmacophore Fragment library contains 985 fragment small molecules.

Pack Size		Price
1 mg	USD	11,183.00
5 mg	USD	26,262.00
10 mg	USD	35,356.00

High Solubility Polyfunctional Group Fragment Library

Catalog No. L7810 — 1159 compounds

The design principle of the highly soluble multifunctional fragment library is to allow rapid, cheap follow-up synthesis to provide quick SAR data. Poised fragments contain at least one functional group which can be synthesised using a robust, well-characterised reaction. Reactions include amide couplings, Suzuki-type aryl-aryl couplings and reductive aminations. Highly soluble multifunctional fragment library contains 1159 kinds of fragment molecules.

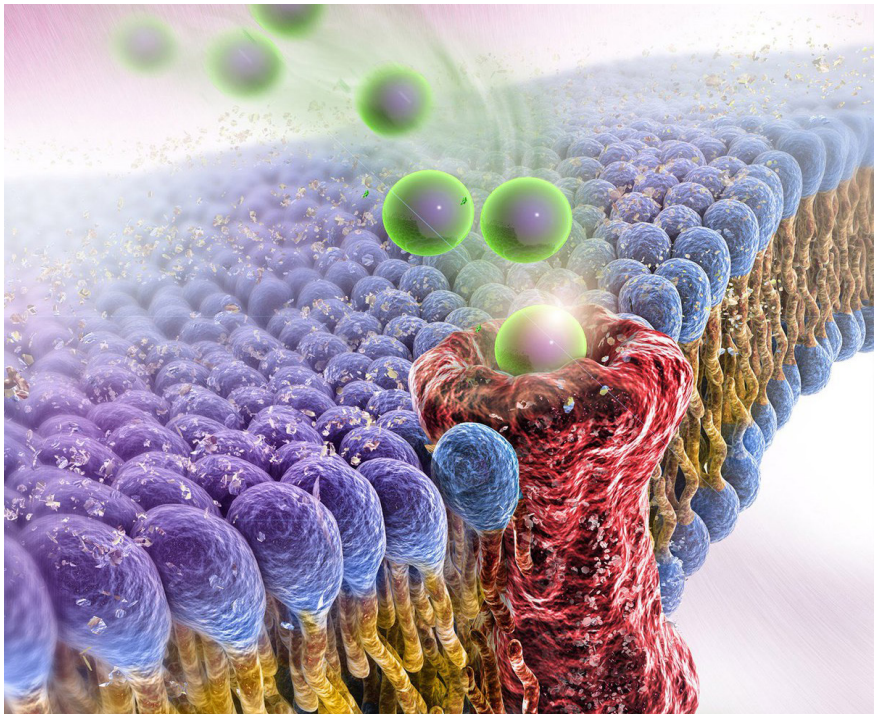
Pack Size		Price
1 mg	USD	12,105.00
5 mg	USD	28,430.00
10 mg	USD	38,273.00

Mini Electrophilic Heterocyclic Fragment Library

Catalog No. L7860 — 371 compounds

Since screening electrophilic fragments has become a promising alternative to discovering and verifying new targets and generating viable chemical starting points, we designed a Mini Electrophilic Heterocyclic Fragment Library. These compounds are basically covalent MiniFrags, containing five- and six-membered nitrogen-containing heterocycles with electron-withdrawing properties that can activate small electrophilic substituents (halogen, ethynyl, vinyl, and nitrile groups). The library contains not only small electrophilic heterocycles, but also N-quaternized analogs with increased reactivity. 371 compounds in total in the Highly Solubility Covalent Heterocyclic Fragment Library

Pack Size		Price
1 mg	USD	4,380.00
5 mg	USD	10,287.00
10 mg	USD	13,849.00



Drug-Fragment Library

Catalog No. L8800 — 1159 compounds

Fragment-based drug discovery (FBDD) has emerged in the past decade as a powerful tool for discovering drug leads. FBDD has played a role in discovery of 3 approved drugs (Vemurafenib, Venetoclax, and Erdafitinib) and at least 30 drugs that are in various stages of clinical development. A fragment-based approach is particularly valuable for more challenging classes of new targets (or "undruggable" targets) where more conventional screening (HTS) has already failed.
Drug-like compounds are often composed of several segmental fragments, any one substructure of a molecule could have affinity for a subpocket fingerprint shared between two or more proteins. There is a significant structure-activity relationship between fragment structure and drug properties. It is easier to find a small molecule that complements a particular subsite within a binding site than a larger molecule that is complementary to the entire site; thus, FBDD usually yields higher hit rates than HTS. In addition, it is easier for fragment optimization to generate leads with improved ADME profile by merging, linking or growing fragments.
It is commonly recognized that high-quality fragment library can increase the FBDD screening hit rate. To meet researchers' expectations, Targetmol® created a Drug-Fragment Library consisting of 1159 fragments arising from the smart fragmentation of 2080 approved drugs and 1100 clinical compounds by structure review and applying many layers of industry recommended medchem filters, including PAINS.

Pack size		Price
100 µL * 10 mM (in DMSO)	USD	8,036.00
1 mg	USD	12,436.00
5 mg	USD	22,322.00
10 mg	USD	31,313.00

Golden Scaffold Library

Catalog No. L5610 — 10000 compounds

While sourcing from 1, 600, 000 drug-like compounds, TargetMol®'s Golden Scaffolds Library of 10,000 compounds was specifically designed for small-scale HTS, with both efficiency and efficacy balanced with 1-3 different functional groups around each scaffold in this library, both chemical space coverage and success rate of screening will be increased.

Pack size		Price
100 µL * 10 mM (in DMSO)	USD	39,024.00
250 µL * 10 mM (in DMSO)	USD	48,780.00

Mini Scaffold Library

Catalog No. L5600 — 5033 compounds

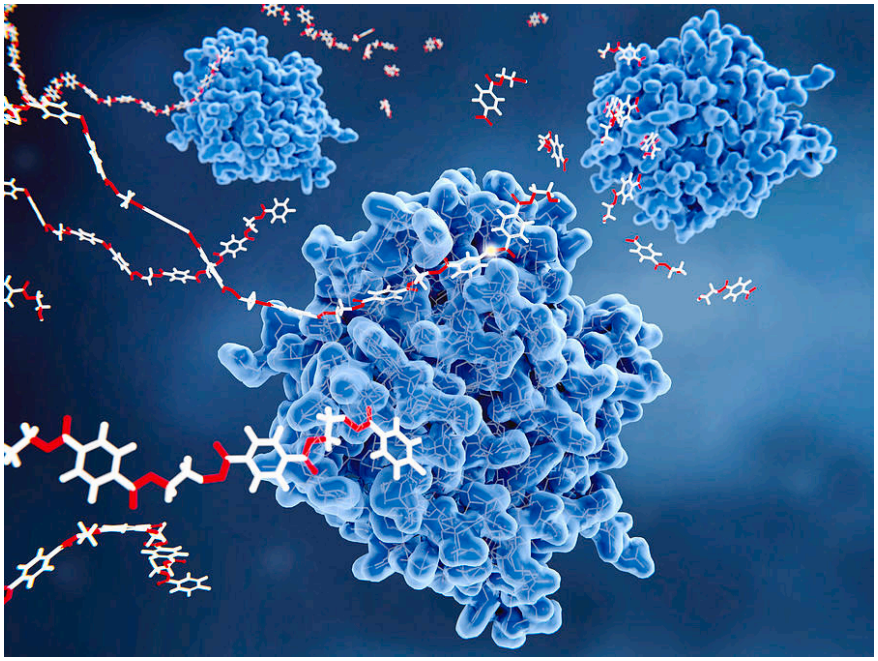
In order to decrease the cost of screening and lower the screening threshold for single project team, TargetMol®'s Mini Scaffolds Library was designed to only include 1 compound for each chemical scaffold and collect 5033 compounds, representing 5033 scaffolds, from a large drug-like chemical source.

Pack size		Price
100 µL * 10 mM (in DMSO)	USD	26,373.00
250 µL * 10 mM (in DMSO)	USD	42,494.00

Pharmacophore-Based Scaffold Library

Catalog No. L5000 — 5000 compounds

TargetMol® first analyzed and constructed pharmacophore models for FDA-approved and clinical-phase small molecular drugs. From millions of scaffolds, each having a molecular weight less than 300, a Pharmacophore-based Scaffold Library was formed by 5000 potentially active drug scaffolds carefully selected using pharmacophore comparison, PAINS removal, and cluster analysis.
Using these scaffolds, we can quickly obtain active lead compounds with novel structures and excellent drug properties.
Pharmacophore-based Scaffold Library is a highly effective tool for high-throughput screening, SBDD, FBDD, DEL, etc.



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SCI	$100 Amazon Gift Card or $200 coupon	1 ⩽ IF< 5

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