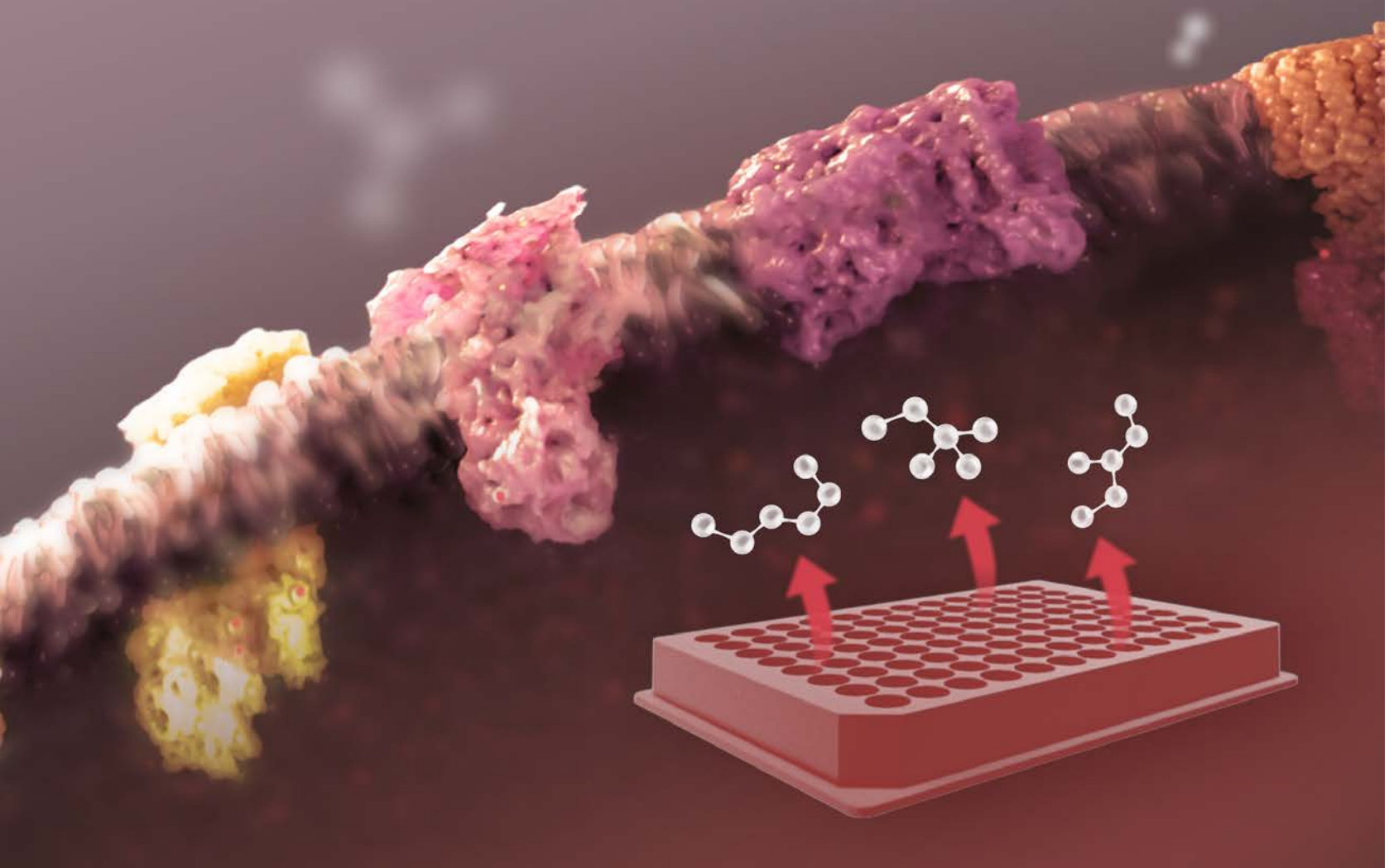
TargetMol®

A DRUG SCREENING EXPERT

COMPOUND LIBRARY

leading your drug discovery Hit-to-Lead



About us

TargetMol Chemicals Inc. is headquartered in the Greater Boston, MA, and specializes in products and services that serve the research needs of chemical and biological scientists worldwide. With a client base in 50+ countries, TargetMol has evolved into one of the biggest global research suppliers for compound libraries and tool compounds. TargetMol diligently updates and offers over 200 types of compound libraries and a wide range of high quality research-used tool compounds, including inhibitors, activators, natural products, peptides, antibodies, and novel life-science kits for laboratory and scientific use. In addition, our lab allows us to conduct CADD (computer-aided drug design) and chemical synthesis to meet the customization needs of our clients.With our high-quality products & services, fast & efficient global supply chain, and professional technical support, we believe we will help you shorten your research process and yield a more successful result.

Compound Libraries

A compound library is a collection of small molecule compounds assembled based on specific characteristics, usually used as a tool for high-throughput screening and drug discovery, assisting in the identification of lead compounds.

Our Advantages

Clear Classification
200+ compound libraries are provided with clear classification and detailed information.

Continuous Update
The compound libraries are updated continuously with average 30% increase each year.

Customization
selectable compounds, quantities, format, plate map, and concentration to form your own library.

Citations:
TargetMol has earned an award for a fast increase in the number of citations in the past year.

Cite us and get rewarded!

Publications	Redemption Option	Impact Factor (IF)
Science/ Nature/ Cell	$300 Amazon Gift Card or $600 coupon	/
SCI	$150 Amazon Gift Card or $300 coupon	IF ≥ 10
SCI	$100 Amazon Gift Card or $200 coupon	5 ≤ IF< 10
SCI	$50 Amazon Gift Card or $100 coupon	1 ≤ IF< 5

For further information, please visit **www.targetmol.com** or contact **inquiry@targetmol.com**

TargetMol® reserves the right to modify or cancel the program at any time.
*All products are for research use only. Not for human or veterinary or therapeutic use.

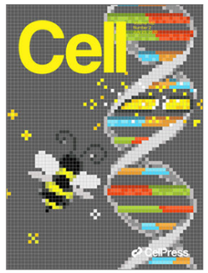
Science
VOLUME 368 ISSUE 6497, 19 JUN 2020

Nature
Volume 582 Issue 7811, 11 June 2020

Nature
2021 592(7854) 469-473

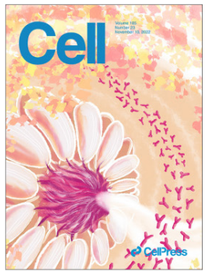
Nature
2020 588(7838) 479-484

Nature
2022, 609(7928) 854-859



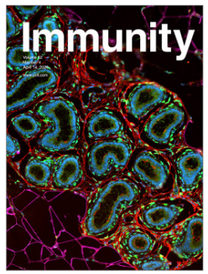
Cell
VOLUME 182, ISSUE 2, P417-428. E13, JULY 23, 2020

Cancer Cell
2020, 38(5) 734-747. e9



Cell
2022, 185(23): 4361-4375. e19

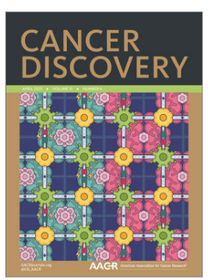
Immunity
2021 54(6) 1123-1136. e8.-22.553



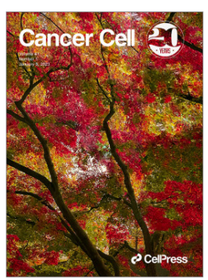
Immunity
2020 52(4) 620-634. e6

Immunity
55(9), 1594-1608.e6.

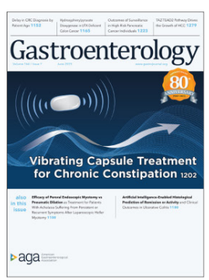
Cell Research
33(1), 46-54



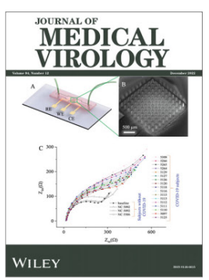
Cancer Discovery
12(2), 356-371



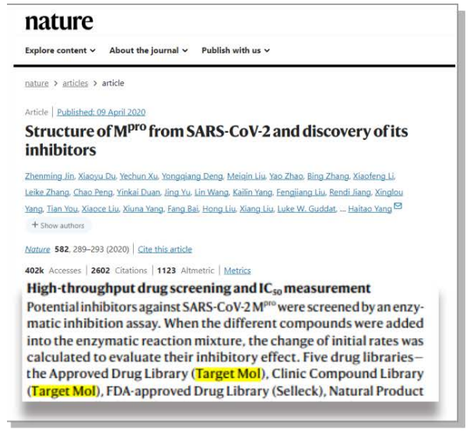
Cancer Cell
Volume 41, Issue 1, p181-195

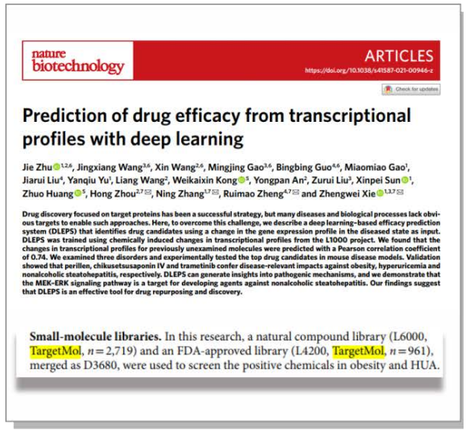


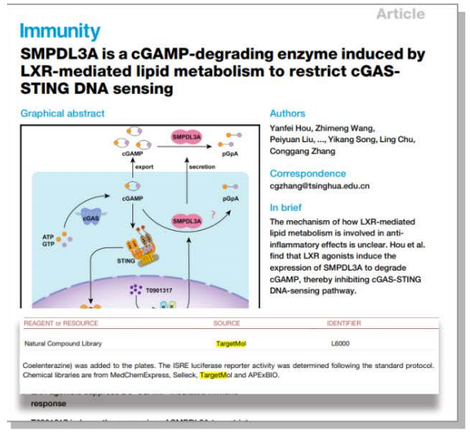
Gastroenterology
Volume 164, Issue 7, p1232 -1247

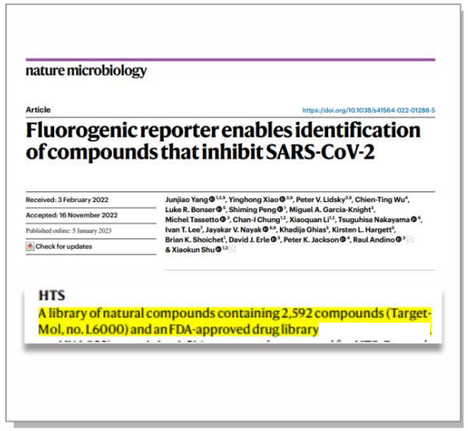


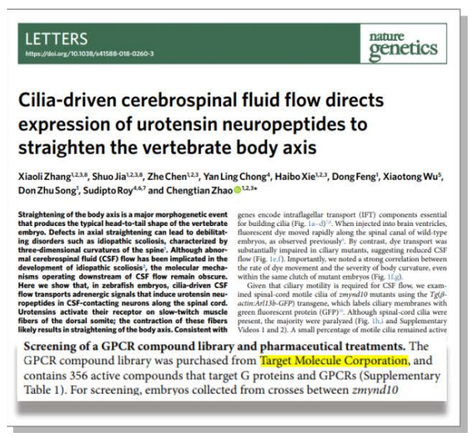
Journal of Medical Virology
Volume 94, Number 12, Dec 2022

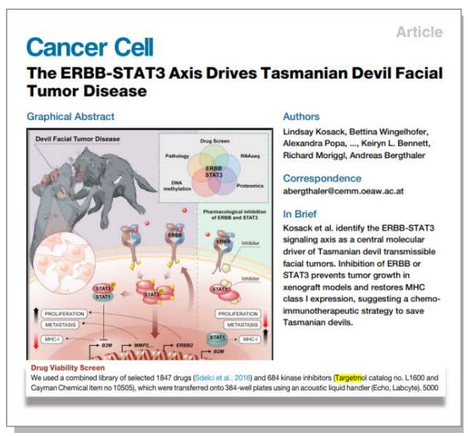












I Focused Bioactive Libraries

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

1.1 Recommended Bioactive Libraries

1.2 Approved/Repurposing Libraries

1.3 Disease-Focused Libraries

1.4 Target/Pathway-Focused Libraries

1.5 Characteristic Bioactive Libraries

II Natural Product Libraries

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

2.1 General Natural Product Libraries

2.2 Characteristic Natural Product Libraries

2.3 Natural Product Libraries for CADD

III Fragment Libraries

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

3.1 General Fragment Libraries

3.2 Characteristic Fragment Libraries

IV Drug-Like Compound Libraries

For drug design and new drug discovery.

4.1 Compound Libraries for HTS/HCS

L5600 Mini Scaffold Library **pg. 50**

L5610 Golden Scaffold Library **pg. 50**

V Custom Library

You can select compounds, quantities, format (dry/solid or DMSO), plate map, and concentration to meet your specific requirement.

Please contact us at inquiry@targetmol.com to customize your library.

Select

Compounds:
Name your desired types of compounds.

Quantity:
Choose among 1 mg, 30 μL * 10 mM (in DMSO), 50 μL * 10 mM (in DMSO), 100 μL * 10 mM (in DMSO), 250 μL * 10 mM (in DMSO). For fragment libraries, the specifications usually comprise 1 mg, 5 mg, and 10 mg.

Lay Out:
96-well plates, 96 2D barcoded tubes, 384-well plates, Echo 384-well microplates (LDV), etc.

Concentration:
In addition to the standard 10 mM concentration, 1 mM, 5 mM, 25 mM, 50 mM, 100 mM, etc. are also available.

Format:
Decide how your compound would be like—— Dry/Solid or DMSO.

Voila! Now sit back and wait for your customized library to be delivered.

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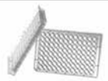
Documentation for TargetMol® Compound Library

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, plate or box ID, column location, row location, coordinates(column and row locations combined), molecular weight, 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 Configuration	96 tubes	96 wells	384 wells	384 wells (Echo)
Capacity (Metric)	1.4 mL	0.34 mL	0.24 mL	12 μL
Material	Polypropylene	Polypropylene	Polypropylene	Cyclic Olefin Copolymer (COC)
Well Shape	V Bottom	V shape	V shape	Flat
Barcode	2D barcoded	-	-	Non-barcoded
Sterility	Non-sterile			
Sealing method	SepraSeal	Heat sealable film /Aluminum Sealing Film	Heat sealable film /Aluminum Sealing Film	Heat seal and MicroClime Environmental Lid compatible
Shipping	Ice Pack/Dry Ice			
Storage	Dry solid: 4°C; Solutions: -80°C or -20°C			
Attention	Avoid repeated freezing and thawing			

For more types of plates, please contact us!

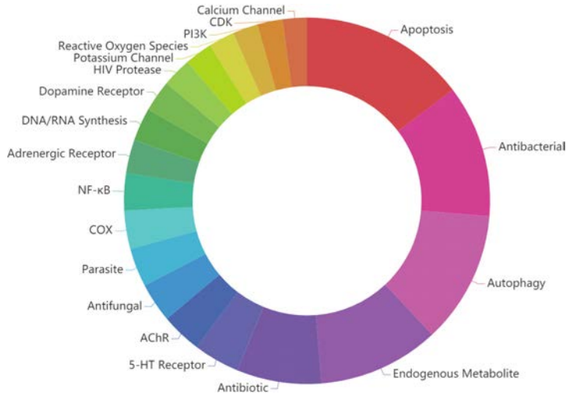
Recommended Bioactive Libraries

Bioactive Compound Library

Catalog No. L4000 — 14,590 compounds

It contains more than 14590 small molecule compounds, with known biological activities causing biological reaction in cells, tissue even whole body, including Clinical compound library (L3400), Preclinical compound library (L3410), and Approved drug library (L1000). All compounds have clear targets and detailed information description, which is the key point to drug research and development like drug repurposing, small molecule inducing stem cell differentiation, and target identification in mechanism interrogation.

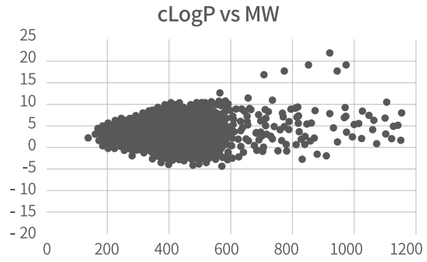
Many scientists have identified small molecules that can regulate cell fate and function, and stem cell differentiation by screening annotated bioactive compound library with confirmed activity and known targets. Recent advances in iPSC technology have made reprogramming of somatic cells towards pluripotency 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 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.

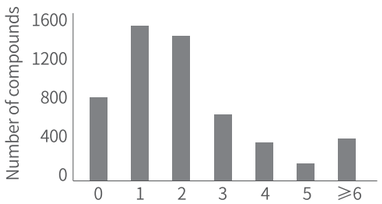


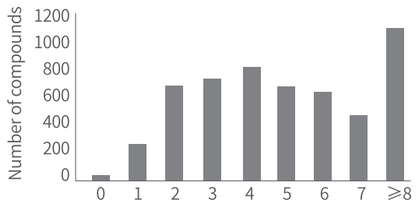
Drug-Like Properties

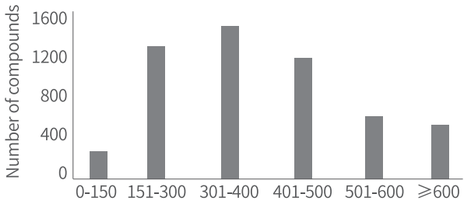
% of compounds compliant with Lipinski' s Rules

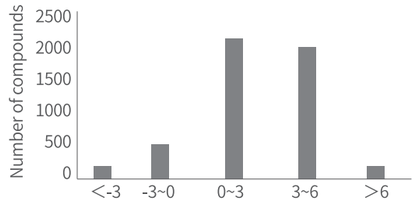
PhysChem Properties	% Compounds
<5 H-Bond donors	89
<10 H-Bond acceptors	89
cLogP<5	89
MW<500	80











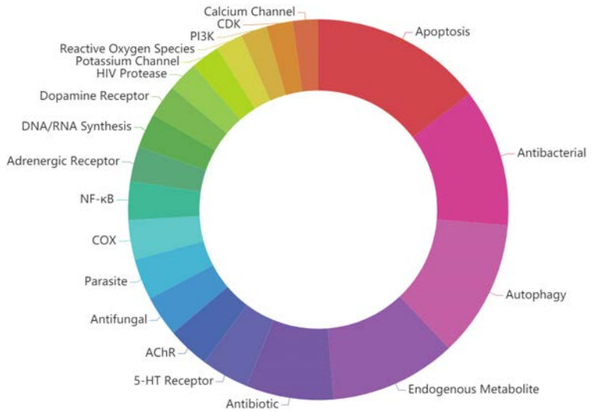
Bioactive Compounds Library Max

Catalog No. L4010 — 22,706 compounds

Bioactive Compound Library Max is a collection of 22706 compounds with biological activity that elicit biological responses in cells, tissues and even individuals. It includes drug molecules that are in preclinical studies, clinical-phase studies and those that are already on the market. With clear targets and comprehensive information, it is ideal for drug repurposing, cell induction and differentiation, and protein target identification in biochemical mechanistic studies.

Because of the clear activity and known targets, many scientists will select small molecules from the Bioactive Compound Library that can be used for cell induction and differentiation. By the combined actions of a single or several small molecules, molecules capable of inducing various somatic cells into induced pluripotent stem cells, neural precursor cells, cardiomyocytes, etc. have been screened; there have even been successful trials of induced differentiation in vivo using combinations of small molecules.

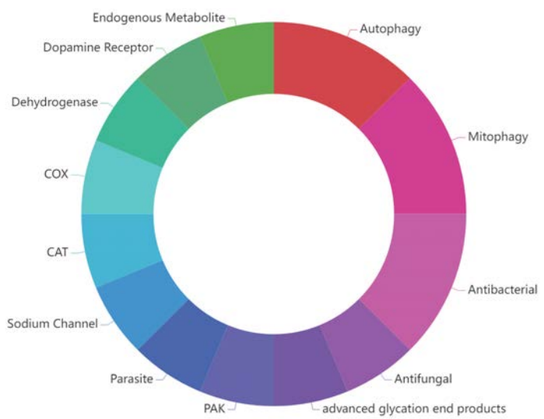
The Bioactive Compound Library Max is a more extensive version of the Bioactive Compound Library (L4000), with the addition of TargetMol's unique and novel compounds (Part C), all of which have clear targets and have been tested for activity at the cellular level. Therefore, it has more novel structures than approved drug libraries and leads to easier active compounds discovery than drug-like compound libraries.



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.

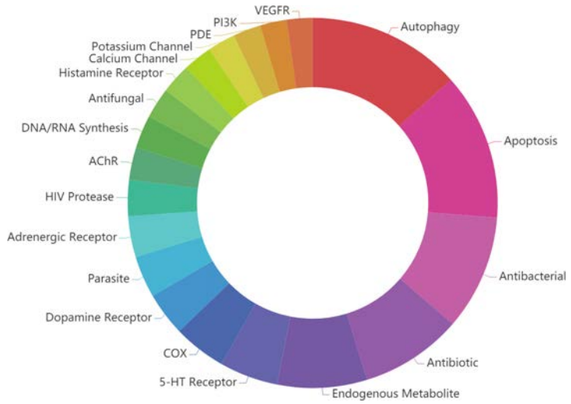


ReFRAME Related Library

Catalog No. L9230 — 3,274 compounds

In 2018 Jeff Janes and his team constructed and published the ReFRAME library through data mining and literature research in the Proceedings of the National Academy of Sciences (PNAS). The team explained the application and utility of the ReFRAME library, where most of the compounds in the library have passed clinical trials Phase I with demonstrated safety profiles, which will significantly shorten the time to of drug candidates to enter clinical trials, reduce the risk of failure, and can be efficiently applied to early-stage drug development screening and discovery of lead compounds. The authors share the ReFRAME library on the Open Data Portal (https://reframedb.org) with the aim of facilitating data sharing and drug discovery opportunities. The Global Center for Health Drug Development (GHDDI), founded by the Gates Foundation and Tsinghua University, has also applied the ReFRAME library to anti-COVID-19 drug discovery.

TargetMol has compiled a library of 3274 ReFRAME compounds, which is a useful tool for drug repurposing and anti-COVID-19 drug development.



Approved/Repurposing Libraries

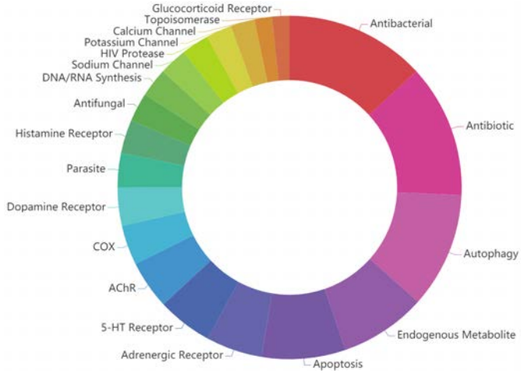
Approved Drug Library

Catalog No. L1000 — 2,863 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 getting complex, the cost of developing new drugs is keeping skyrocket. Drug repositioning, also known as old drugs for new uses, is an effective strategy to find new indications for existing drugs and has recently drawn attention and has led to several blockbuster drugs because of its high efficiency and low-cost. High-content screens, new biomarkers, noninvasive imaging techniques, and advanced in bioinformatics have created new opportunities for pursuing novel indications for approved compounds.

Approved drugs all have known and well-characterized bioactivities, safety and bioavailability – properties which could dramatically accelerate drug development and optimization. Hits from this set will provide a significant head start in any drug optimization program.

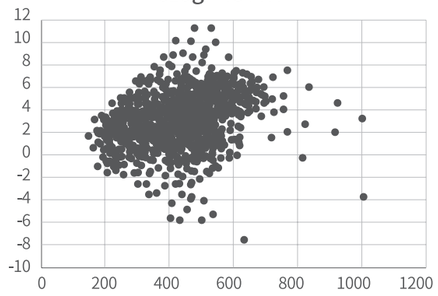
In addition, a growing number of compounds have been identified from this library that can functionally replace reprogramming transcription factors, enhance efficiency of iPSC generation and accelerate the reprogramming process by single use or a combination of several molecules.

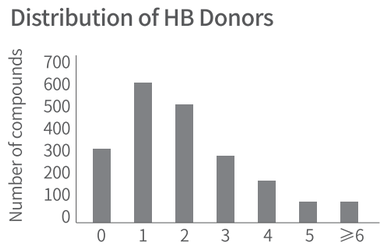


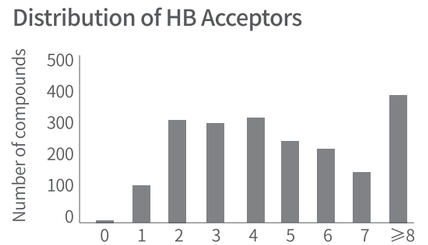
Drug-Like Properties

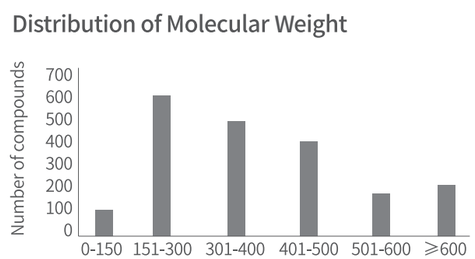
% of compounds compliant with Lipinski' s Rules

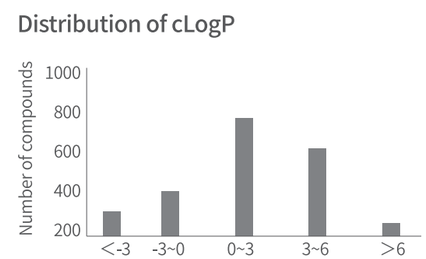
PhysChem Properties	% Compounds
<5 H-Bond donors	88
<10 H-Bond acceptors	90
cLogP<5	90
MW<500	79









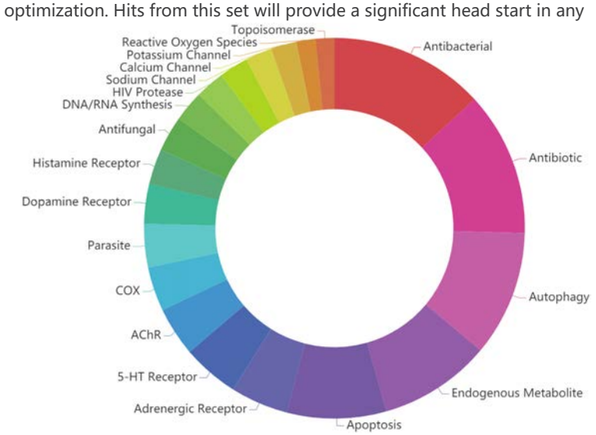


FDA-Approved & Pharmacopeia Drug Library

Catalog No. L1010 — 3,158 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 getting complex, the cost of developing new drugs is keeping skyrocket. Drug repositioning, also known as old drugs for new uses, is an effective strategy to find new indications for existing drugs and has recently drawn attention and has led to several blockbuster drugs because of its high efficiency and low-cost. High-content screens, new biomarkers, noninvasive imaging techniques, and advanced in bioinformatics have created new opportunities for pursuing novel indications for approved compounds.

Approved drugs all have known and well-characterized bioactivities, safety and bioavailability – properties which 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 efficiency of iPSC generation and accelerate the reprogramming process by single use or a combination of several molecules.

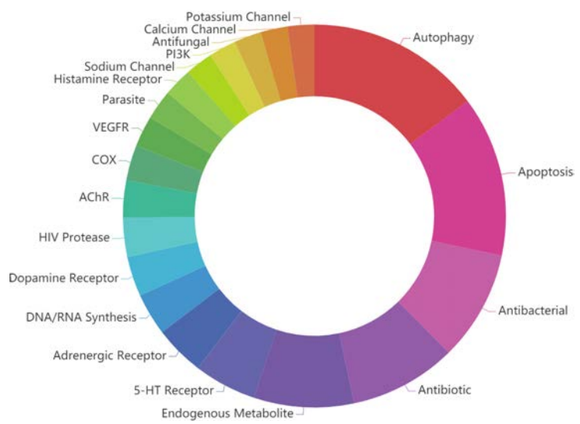


TargetMol's FDA-Approved & Pharmacopeia Drug Library collects 3158 compounds from approved institutions such as FDA, EMA, PMDA, NMPA, etc. or pharmacopoeia such as USP, BP, JP, etc., which can be used for drug repositioning and cell induction.

Clinical Compound Library

Catalog No. L3400 — 3,480 compounds

Clinical compound library is a collection of 3480 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 pre-clinical evidence.

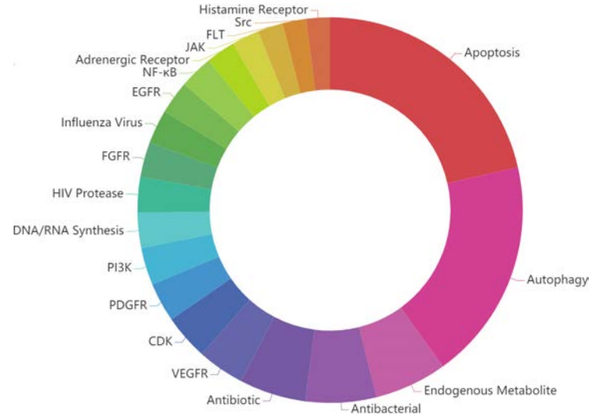


Every compound contains detailed information on pharmacological activities, targets, clinical development status, and indications with broad spectrum covering several therapeutic areas from cancer, inflammation, infection, neuropsychiatry to cardiology, and many drug targets such as JAK, EGFR, mTOR, CDK, HDAC, AKT, PARP, etc. It is an effective tool for drug screening as well as for cell differentiation induction.

Preclinical Compound Library

Catalog No. L3410 — 709 compounds

Preclinical Compound Library is a collection of 709 compounds that are in preclinical phase with clear targets and detailed information on disease indication and reference.

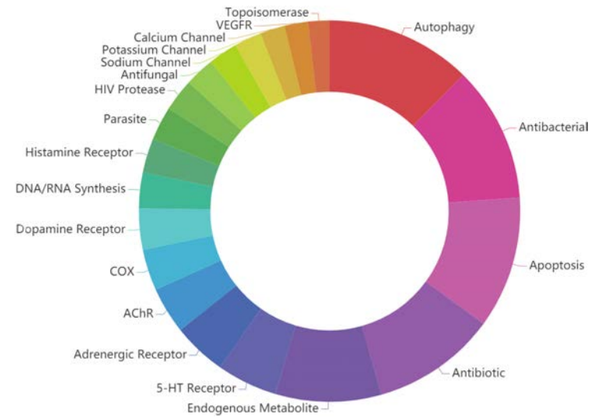


Drug Repurposing Compound Library

Catalog No. L9200 — 4,330 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 getting complex, the cost of developing new drugs is keeping skyrocket. Drug repositioning, also known as old drugs for new uses, is an effective strategy to find new indications for existing drugs and has recently drawn attention and has led to several blockbuster drugs because of its high efficiency and low-cost. High-content screens, new biomarkers, noninvasive imaging techniques, and advanced in bioinformatics have created new opportunities for pursuing novel indications for approved compounds.

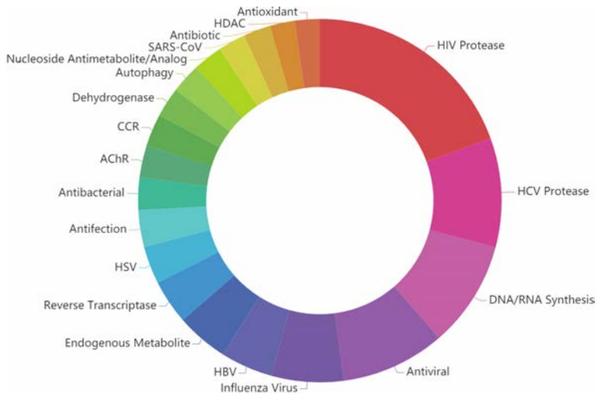
The Drug Repurposing Compound Library by TargetMol, containing 4330 approved and clinical drugs, which have undergone extensive preclinical studies and have well-characterized bioactivities, safety and bioavailability – properties which could dramatically accelerate drug development and optimization, is a good tool for drug repurposing and cell induction.



Disease-Focused Libraries

Anti-Viral Compound Library
Catalog No. L1700 — 1,040 compounds

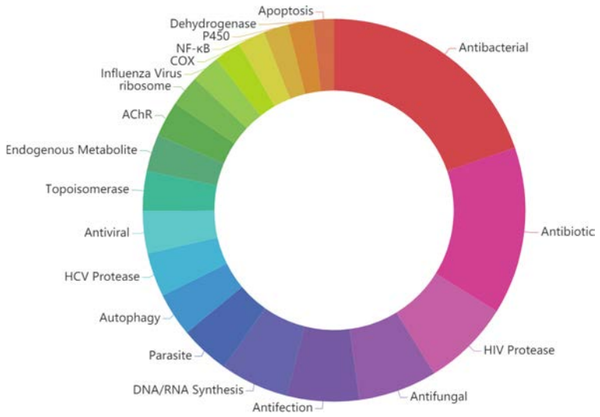
Virus is a small infectious agent that replicates only inside the living cells of other organisms through various pathways, and causes the damage to the host cells. Common diseases caused by virus include smallpox, the common cold, chickenpox, influenza, shingles, hanta fever, herpes, etc. AIDS, polio, 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 1040 compounds with anti-virus bioactivity, and is an appropriate tool for drug repurposing for new anti-virus drug discovery based on the fact that these viruses rely on common host cellular mechanisms to promote discrete stages of their life cycles.

Anti-Infection Compound Library
Catalog No. L1800 — 2,977 compounds

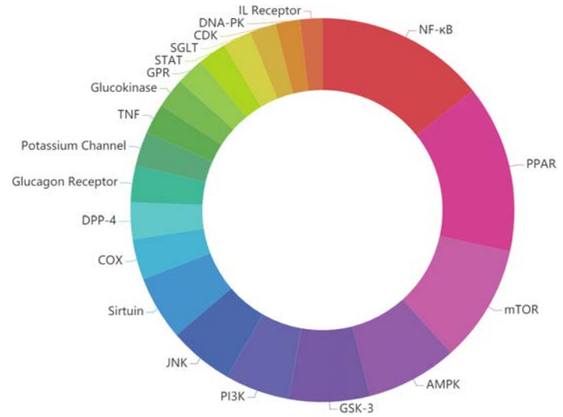
An infection happens when a foreign organism enters a person's body and causes harm. These infectious organisms are known as pathogens. Examples of pathogens include bacteria, viruses, fungi, prions, and parasites. Some infections are mild and barely noticeable, but others are severe and life-threatening, and some are resistant to treatment.



A unique collection of 2977 bioactive small molecules with anti-bacterial, anti-virus, and anti-parasite capability was carefully selected by TargetMol for high throughput drug screening and new drug target identification in anti-infection research.

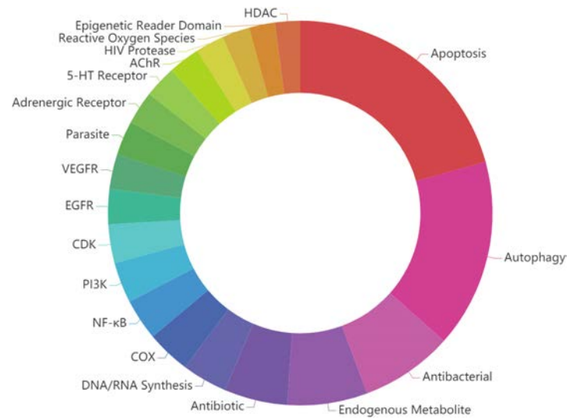
Anti-Diabetic Compound Library
Catalog No. L1900 — 690 compounds

Diabetes is a chronic, metabolic disease characterized by elevated levels of blood glucose (or blood sugar). Too much sugar in the blood for a long 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 to diabetes but people with diabetes can stay healthy by managing their disease through diet and the help of medicine. A unique collection of 690 small molecules affecting the development of diabetes is an effective tool for diabetes research and drug screening.



Anti-Cancer Compound Library
Catalog No. L2100 — 7,360 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, causing more damage, and invading 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).

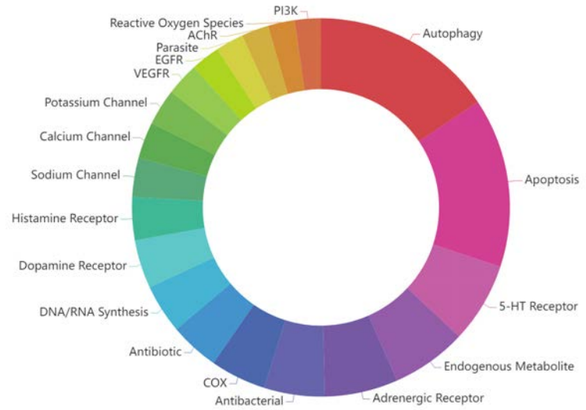


We carefully select 7360 compounds with anti-tumor activity based on different characteristics and abnormal metabolism with cancer cells. All of these compounds are the small molecules modulating the metabolism, growth, invasion, and metastasis of tumor cells that can be used for tumor-related research and anti-tumor drug screening.

Anti-Cancer Drug Library

Catalog No. L2150 — 2,900 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, causing more damage, and invading 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).



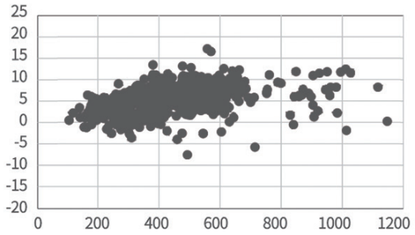
We carefully select 2900 anticancer drugs including FDA approved and compounds in clinical trial phases as Anticancer Drug Library that can be used for tumor-related research and anti-tumor drug screening.

Drug-Like Properties

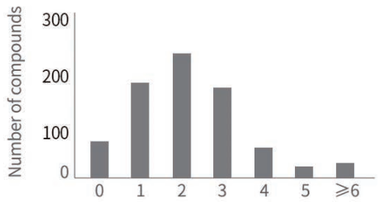
% of compounds compliant with Lipinski' s Rules

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

cLogP vs MW

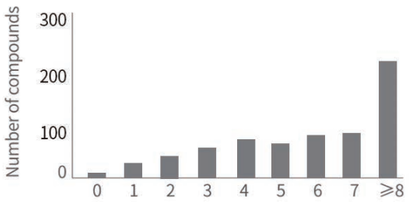


Distribution of HB Donors



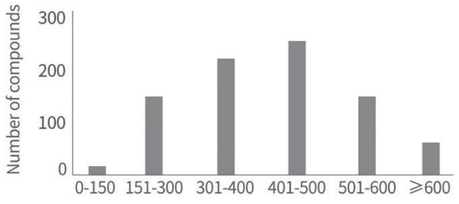
HB Donor

Distribution of HB Acceptors



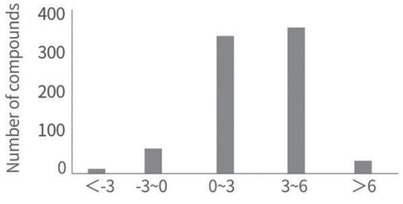
HB Acceptor

Distribution of Molecular Weight



Molecular Weight

Distribution of cLogP



cLogP

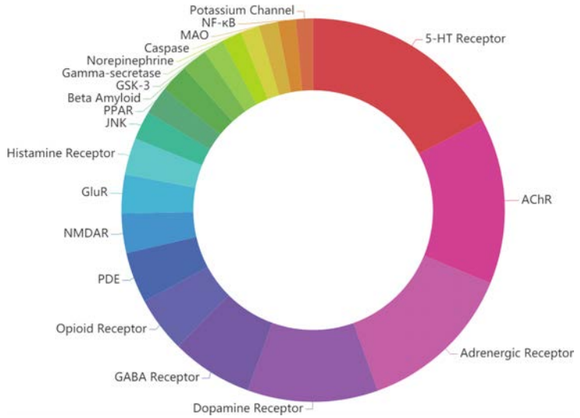
Anti-Neurodegenerative Disease Compound Library

Catalog No. L2620 — 1,622 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 1622 compounds related to neurodegenerative diseases having therapeutic effect or acting on neurodegenerative disease-related targets.

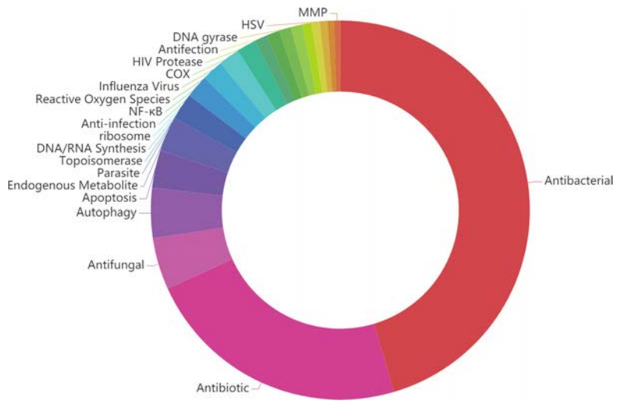


Anti-Bacterial Compound Library

Catalog No. L4520 — 921 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), being 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.

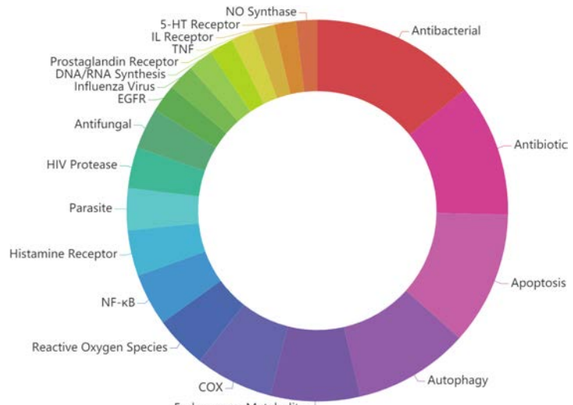
TargetMol's Anti-Bacterial Compound Library consists of 921 small molecules with antibacterial activity, is an effective tool for antibiotics and antibacterial drug development.



Immunology/Inflammation Compound Library

Catalog No. L4700 — 3,483 compounds

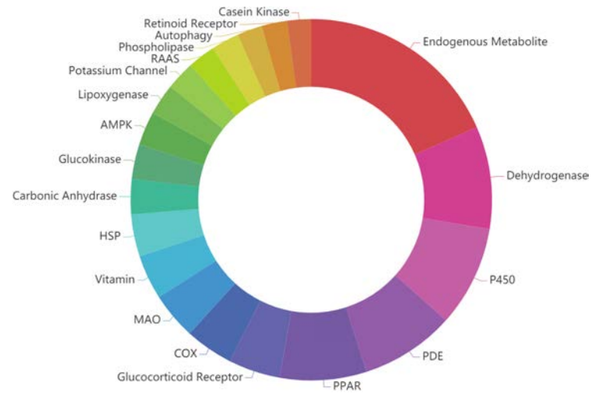
An autoimmune disorder occurs when the body's immune system attacks and destroys healthy body tissue by mistake. Areas often affected by autoimmune disorders include blood vessels, connective tissues, joints, and skin, etc. The chemical advances in the 19th–20th centuries brought about the development of non-steroidal anti-inflammatory drugs (NSAIDs). Although effective in the treatment of inflammatory diseases, NSAIDs have some undesirable and adverse effect, such as ulcers, kidney injury, and bleeding in the gastrointestinal tract. Although initially identified as anti-tumor molecule, TNF is now considered as a pleiotropic cytokine which 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 for 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 the autoimmune inflammatory diseases and chronic inflammatory diseases.



Anti-Metabolism Disease Compound Library

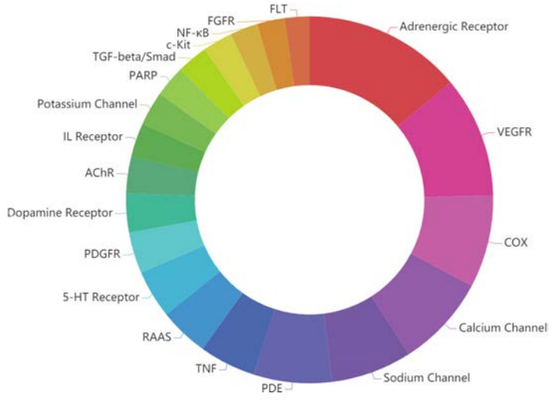
Catalog No.L5200 — 1,558 compounds

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 metabolism research area is the biological regulatory mechanism and its role in obesity, diabetes, cardiovascular diseases, and cancer. The unique collection of 1558 small chemicals targeting metabolism diseases will provide the support for metabolism research and related drug screening.



Anti-Cardiovascular Disease Compound Library
Catalog No. L5400 — 1,428 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.



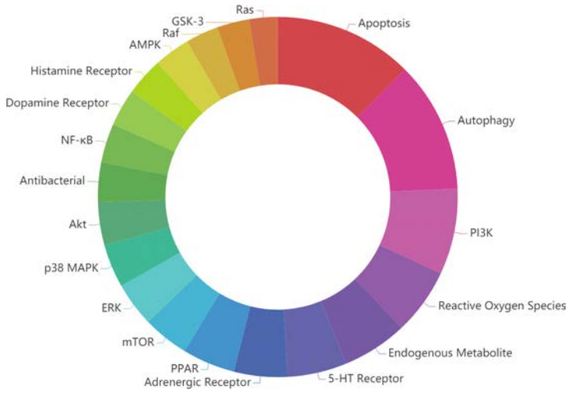
A unique collection of 1428 cardiovascular diseases related compounds by TargetMol can be used for cardiovascular diseases related research and high throughput and high content screening for new drugs.

Anti-Obesity Compound Library
Catalog No. L7100 — 2,286 compounds

Obesity has become the public health issue of the day—and for good reason. 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, multi-factorial 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 treatment 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 anti-obesity drug.Many pharmaceutical companies have invested substantial capital and labor to develop anti-obesity drugs; however, most of the anti-obesity 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 anti-obesity bioactive ingredients from food or drugs, especially by inhibiting intestinal fat absorption, increasing fat cell metabolism, and enhancing the 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.

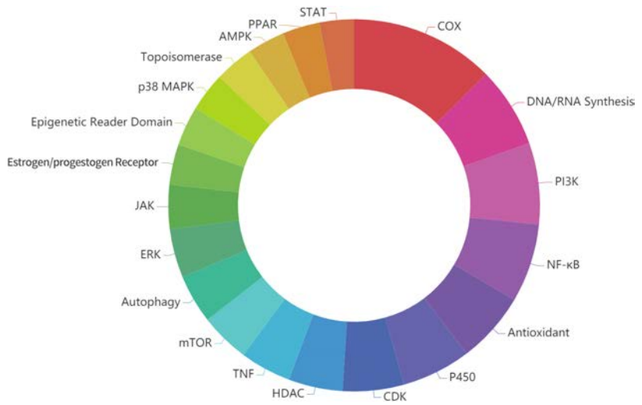
Based on the published literature, TargetMol carefully collects 2286 compounds with anti-obesity activity as Anti-Obesity Compound Library, which can be used for anti-obesity research and drug discovery.



Anti-Aging Compound Library
Catalog No. L8200 — 3,324 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 twelve 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, altered intercellular communication, Chronic inflammation, Dysbiosis, Disabled macroautophagy.

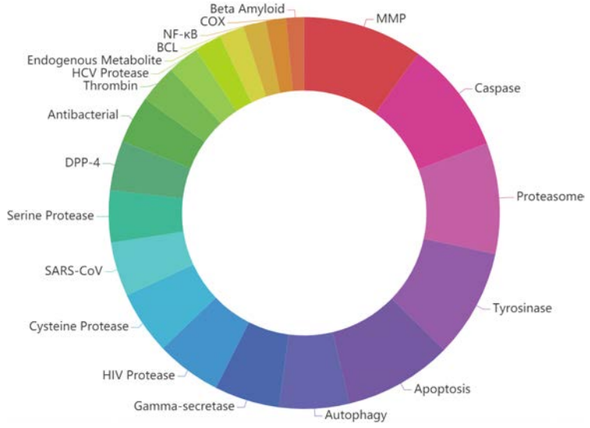
There is great interest in finding drugs capable of extending human lifespan and healthspan. Compounds are sought that are capable of modulating multiple aging pathways, thereby preventing a broad-spectrum of age-related diseases. The TargetMol's Anti-Aging Compound Library, a unique collection of 3324 anti-aging compounds, is an effective tool for anti-aging research, and anti-aging drug screening.



Target/Pathway-Focused Libraries

Protease Inhibitor Library
Catalog No. L1100 — 344 compounds

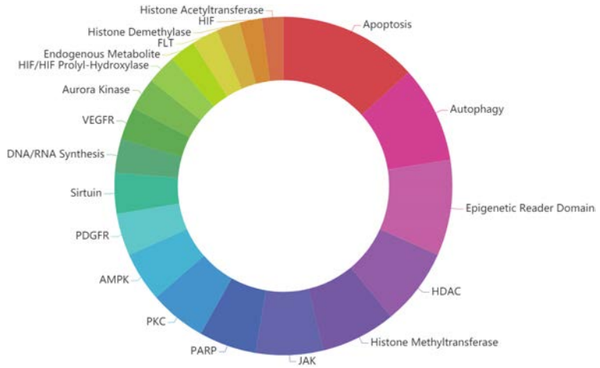
Protease inhibitors are molecules that inhibit the function of proteases (enzymes that aid the breakdown of proteins), including proteins protease inhibitors, natural protease inhibitors, and synthetic protease inhibitors. (1). Antiprotozoal activity: protease inhibitors could be used against malaria 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 344 small protease and proteasome inhibitors, can be used for research in Chemical Genomics and drug screening.

Epigenetics Compound Library
Catalog No. L1200 — 960 compounds

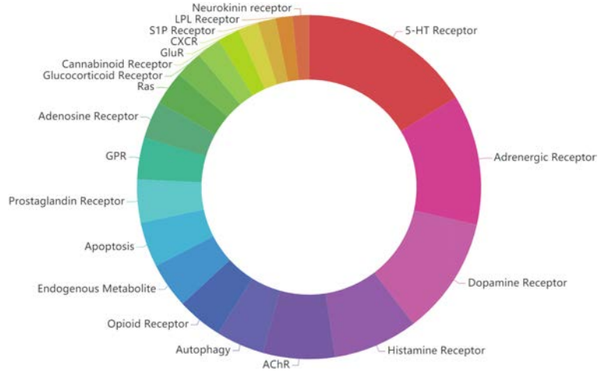
Epigenetics is the study of molecular processes that influence the flow of information between a constant DNA sequence and variable gene expression patterns. This includes investigation of nuclear organization, DNA methylation, histone modification and RNA transcription. Epigenetic processes can result in intergenerational (heritable) effects as well as 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 960 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.

GPCR Compound Library
Catalog No. L1500 — 1,633 compounds

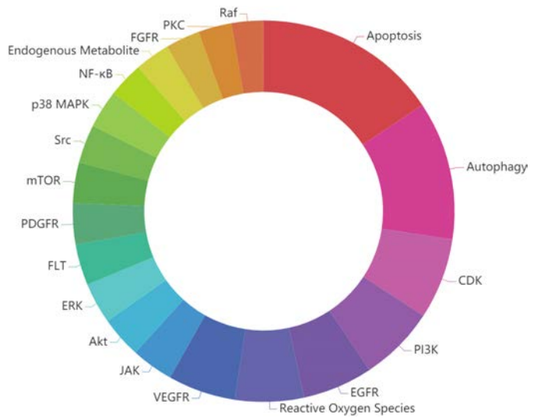
G-protein-coupled receptors (GPCRs) are the largest and most diverse group of membrane receptors in eukaryotes that detect molecules outside the cell and activate internal signal transduction pathways and, ultimately, cellular responses. GPCRs are involved in nearly every aspect of animal life, from 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 campaigns 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, a focused small molecule libraries developed against particular GPCRs containing 1633 GPCR-active agents for GPCR drug discovery.

Kinase Inhibitor Library
Catalog No. L1600 — 2,203 compounds

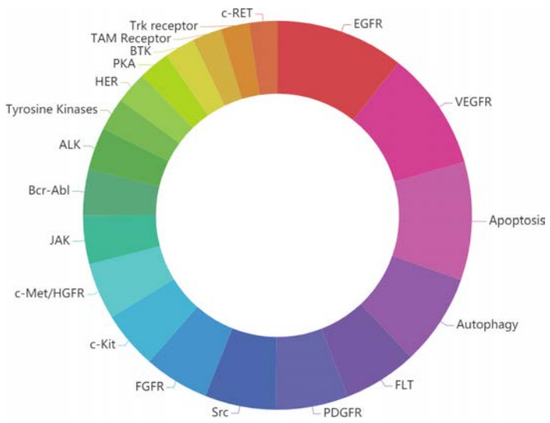
In biochemistry, a kinase is an enzyme that catalyzes the transfer of phosphate groups from high-energy, phosphate-donating molecules (ATP) to specific substrates. This process is known as phosphorylation. The protein kinases make up the majority of all kinases and are widely studied. A protein kinase 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.



Tyrosine Kinase Inhibitor Library
Catalog No. L2200 — 746 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 play a pivotal role in inflammatory diseases such as idiopathic pulmonary fibrosis.

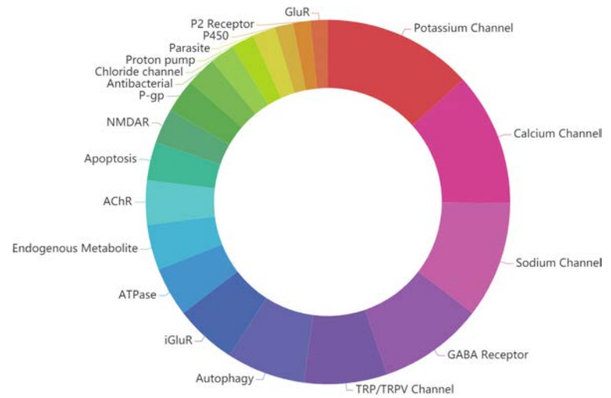
The Tyrosine Kinase Inhibitors Library by TargetMol, containing 746 tyrosine kinase inhibitors, can be used for research in tyrosine kinase signaling, and drug screening for related diseases.



Ion Channel Inhibitor Library
Catalog No. L2300 — 946 compounds

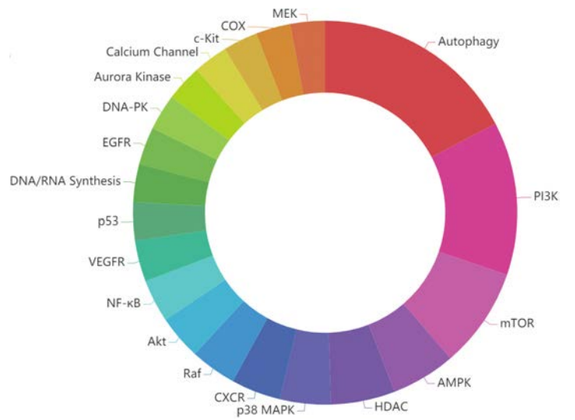
Given the central functional role that the ion channel superfamily plays in human physiology, its membrane localization, and the diverse tissue distribution of different members of the family, it represents an attractive potential target class for drug discovery. Ion channelsplay a fundamental role in 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 946 compounds targeting ion channels, can be used for research in ion channel, high throughput screening and high content screening for ion channel drug discovery.



Autophagy Compound Library
Catalog No. L3200 — 1,248 compounds

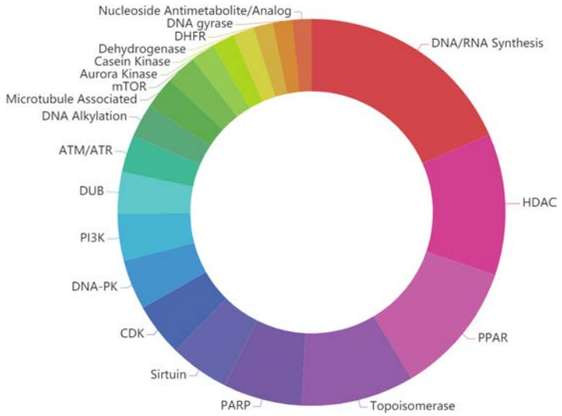
Autophagy is the natural, regulated mechanism of the cell that disassembles unnecessary or dysfunctional components. Targeted damaged cytoplasmic constituents are isolated from the rest of the cell within a double-membraned vesicle known as an autophagosome. The autophagosome eventually fuses with lysosomes and the contents are degraded and recycled. Autophagy, cellular senescence, and apoptosis are three key responses of a cell facing a 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 1248 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.



DNA Damage & Repair Compound Library

Catalog No. L3900 — 937 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 less effective the current therapies with antibiotics. Developing inhibitors of DNA repair and related pathways in pathogens will have utility in the treatment of infections.

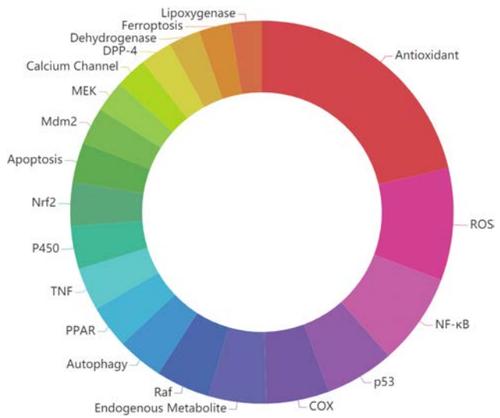


The TargetMol's DNA Damage & Repair Compound Library, a unique collection of 937 DNA Damage & Repair related compounds, can be used for research in DNA damage and repair, and high throughput screening (HTS) and high content screening (HCS).

Ferroptosis Compound Library

Catalog No. L8700 — 800 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.

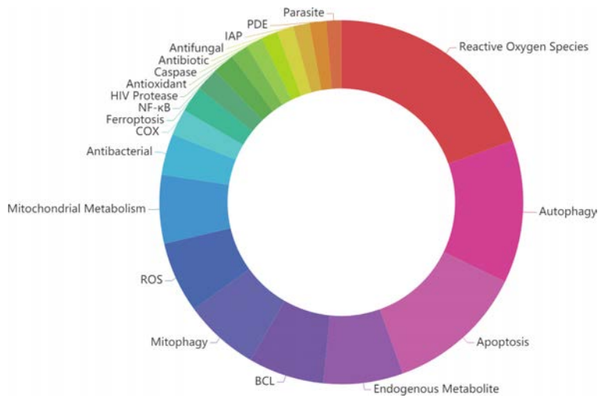


TargetMol collects 800 compounds related to ferroptosis signaling pathway with targets including GPX4, System Xc − , HSPB1, NRF2, VDAC2/3, Ras, TFR1, NOX, p53, CARS, ROS, SLC7A11, etc. Iron chelators and lipid peroxidation inhibitors are also included in this library.

Cuproptosis Compound Library

Catalog No. L8710 — 411 compounds

Copper is an essential cofactor for all organisms, and yet it becomes toxic if concentrations exceed a threshold maintained by evolutionarily conserved homeostatic mechanisms (Tsvetkov et al., 2022). The mechanism of cuproptosis (copper-dependent death), is significantly different from other known cell death such as apoptosis, pyroptosis, necrosis and ferroptosis. Copper-dependent death occurs by means of direct binding of copper to lipoylated components of the tricarboxylic acid (TCA) cycle. This results in lipoylated protein aggregation and subsequent iron-sulfur cluster protein loss, which leads to proteotoxic stress and ultimately cell death (Tsvetkov et al., 2022). Nowadays, cuproptosis has been associated with diseases such as amyotrophic lateral sclerosis (ALS), breast cancer, melanoma, adult neuroblastoma, and prostate cancer.

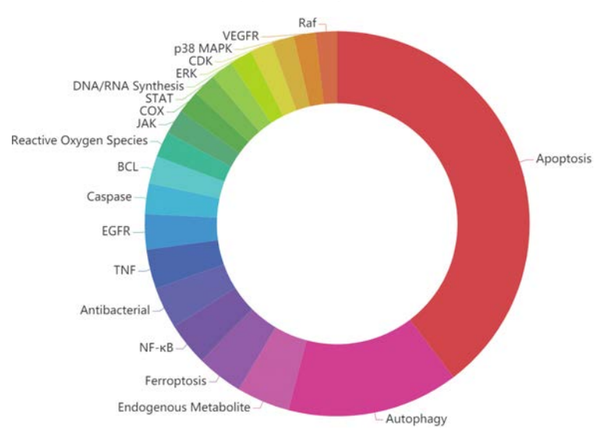


TargetMol's Cuproptosis Compound Library is a collection of 411 compounds related to copper-dependent death that can be used to study its mechanism and related diseases.

Apoptosis Compound Library

Catalog No. L9000 — 1,796 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.

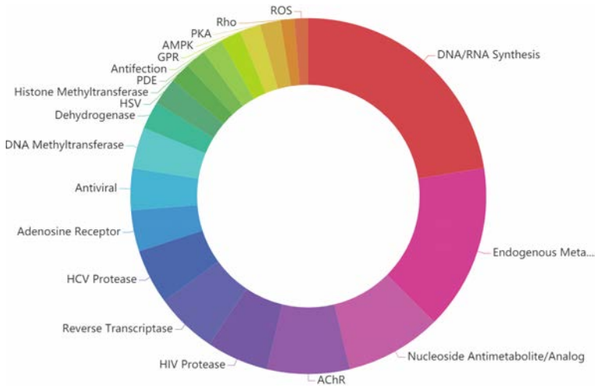


TargetMol's collection of 1796 apoptosis-related compounds, Apoptosis Compound Library, is divided accordingly with compounds designed for either pro- or anti-apoptosis purposes and can be used for research in cancer and neurodegenerative diseases.

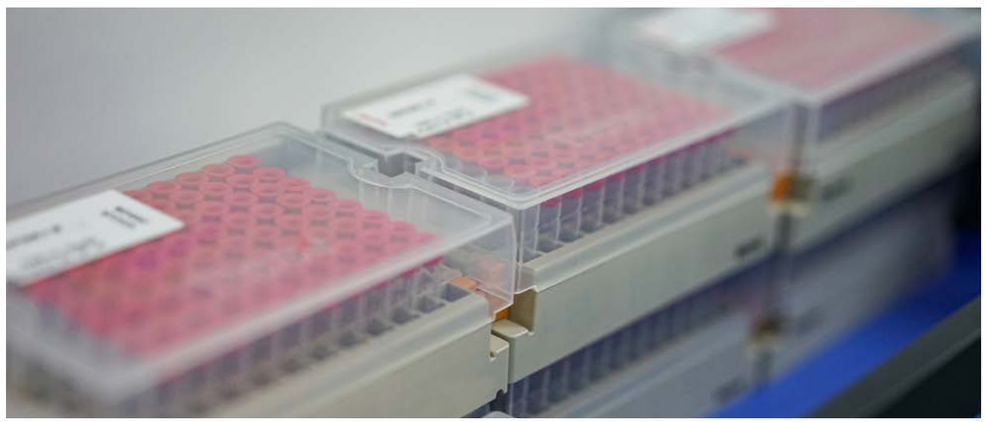
Characteristic Bioactive Libraries

Nucleotide Compound Library
Catalog No. L1720 — 337 compounds

Nucleoside analogues are nucleosides which contain a nucleic acid analogue and a sugar. Nucleotide analogs are nucleotides which contain a nucleic acid analogue, a sugar, and one to three phosphate groups. Nucleoside and nucleotide analogues can be used in therapeutic drugs, include 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 anti-viral drugs, almost 50% are nucleoside or nucleotide analogues. Anti-tumor 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.



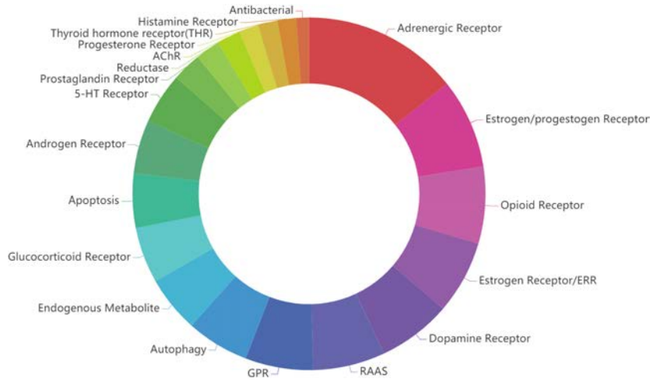
TargetMol's nucleotide compound library collects 337 nucleoside and nucleotide analogues, some of which are in the clinical trial phases or marketed therapeutic drugs, can be used for research and development of anti-viral, anti-tumor, anti-fungal, and anti-depressive drugs.



Endocrinology-Hormone Compound Library
Catalog No. L2400 — 813 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.

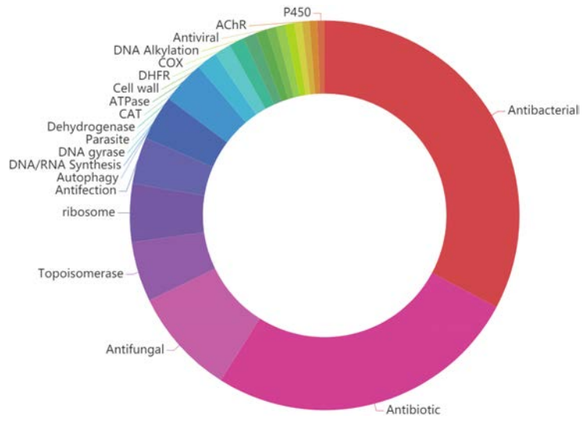
The Endocrinology-Hormones Compound Library by TargetMol, containing 813 compounds targeting endocrine system, can be used for research in endocrine system, high throughput screening and high content screening for new drugs in endocrine diseases.



Antibiotics Library
Catalog No. L4400 — 708 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 708 compounds with antibiotic activity, can be used for antibacterial research and related drug screening.

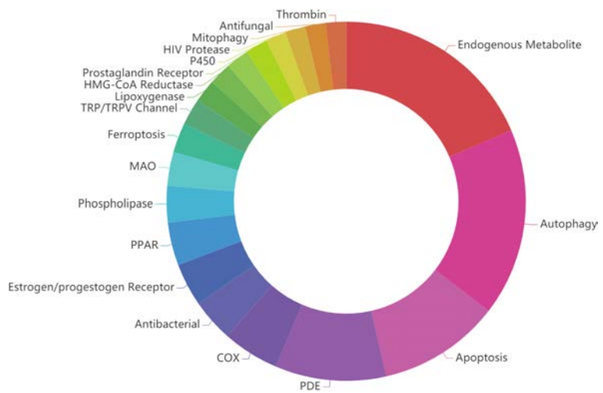


Bioactive Lipid Compound Library

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 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 which 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).

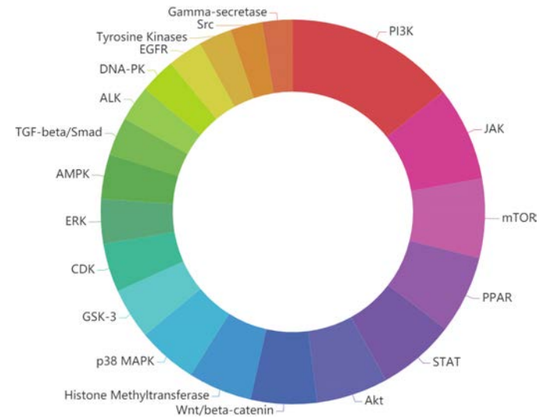


Stem Cell Differentiation Compound Library

Catalog No. L8000 — 1213 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 functional 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 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 1213 stem cell differentiation signaling targeted compounds, can be used for stem cell research and related drug screening (high throughput and high content screening).

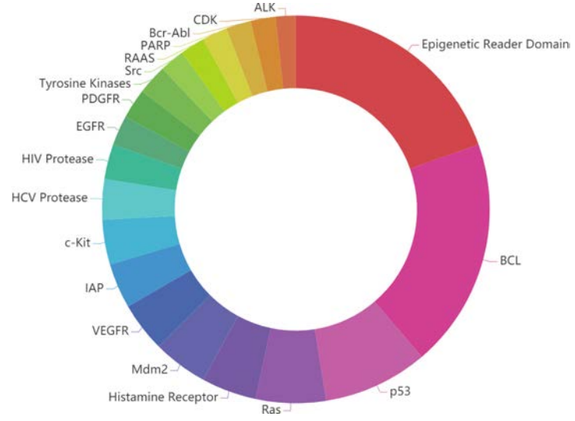


PPI Inhibitor Library

Catalog No. L9400 — 490 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 490 PPI-related compounds, can be used for research on protein-protein interaction.



Covalent Inhibitor Library

Catalog No. L9410 — 1,949 compounds

Covalent inhibitors are small organic molecules which interact with specific target proteins and form a covalent bond, resulting an alteration of the protein conformation and subsequently inhibit 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.

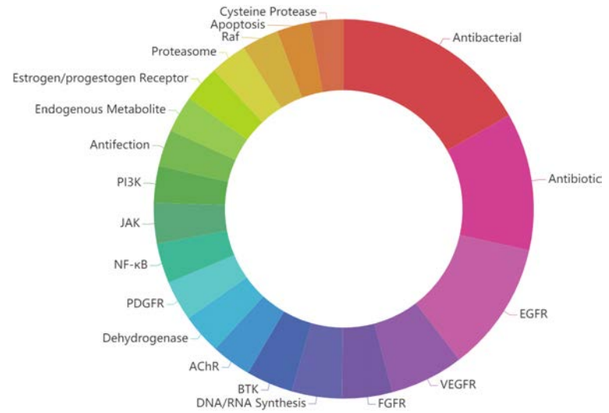
Although the majority of successful covalent drugs were discovered through serendipity in phenotypic screens, and their molecular mechanisms were elucidated afterwards, covalent drugs have made a major impact on human health and have been highly successful drugs for the pharmaceutical industry over the 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 had 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 has 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 1949 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.



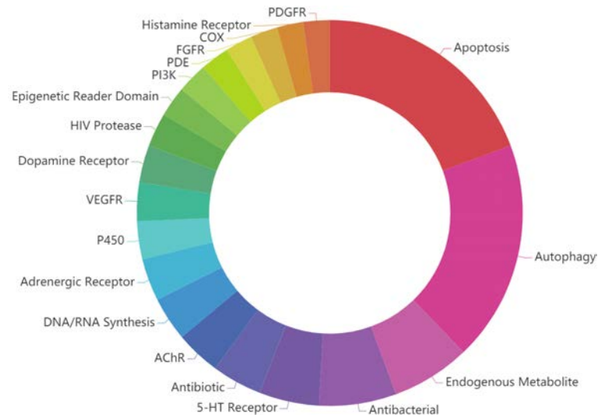
Target-Focused Phenotypic Screening Library

Catalog No. L9500 — 1,832 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.

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 finally was 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.



General Natural Product Libraries

Natural Product Library for HTS
Catalog No. L6000 — 4,320 compounds

Natural products are compounds produced by organisms in nature. Their structures and functions have been selected and optimized during the long evolutionary process of nature, resulting in highly diverse structures through different processes such as oxidation and reduction, rearrangement reaction, cationic cyclization, condensation reactions, and pericyclic reactions.

These unique chemical structures endow natural products with target-specific binding ability and good biological activity. Therefore, natural products have become an important source for drug discovery of major disease treatments. Whenever a new game-changing drug emerges, it is usually, though not every time, accompanied by the discovery of a new type of natural product, which also promotes the development of medicinal chemistry and life sciences.

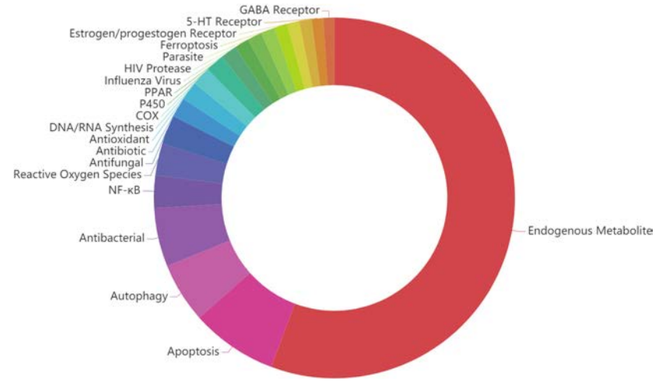
TargetMol's Natural Product Library for HTS has a collection of 4320 carefully selected natural product monomers. These natural product monomers are widely sourced, structurally diversed and highly representative. They exist in natural sources extracted and purified from more than 2,900 kinds of Chinese medicinal herbs, animals and microorganisms, covering more than 500 different scaffolds and more than 1,000 target receptors, and most of the components have reached the purity of reference standards. In addtion, the library also contains many rare natural products with extremely high unit prices, which makes the library highly cost-effective. TargetMol's Natural Product Library for HTS is a powerful tool for drug development, pharmacological research, stem cell differentiation, fingerprint research, quality research and other fields.

Characteristic Natural Product Libraries

Human Endogenous Metabolite Library
Catalog No. L2500 — 508 compounds

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 has 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, saccharide, 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.

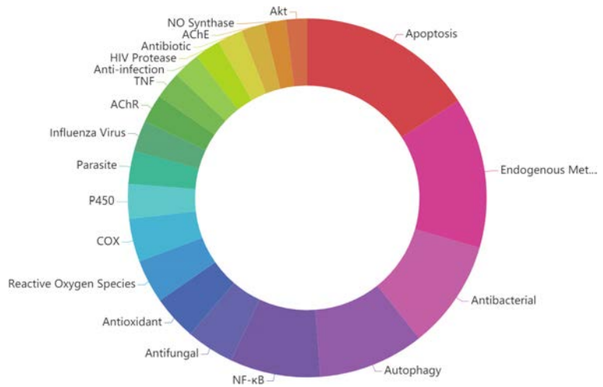
TargetMol's collection of 508 endogenous metabolism-related compounds, Human Endogenous Metabolism Compound Library, can be used for research in endogenous metabolism-related diseases and drug screening.



Selected Plant-Sourced Compound Library

Catalog No. L4600 — 3,075 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 mankind 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 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 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 3075 plant-sourced compounds that can be used for natural drug screening and new drug development.

Mini Fungal Metabolite Natural Product Screening Library

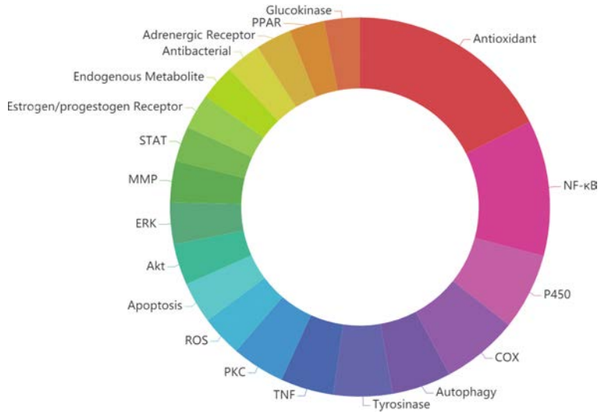
Catalog No. L6001

For thousands of years，natural products produced by organisms in nature have been utilized as medicines. As early as the second century B.C., Artemisia caruifolia was used to treat malaria. In the early modern era, advances in microbiology, particularly Alexander Fleming's discovery of penicillin, have ushered in a new era of drug discovery from microorganisms. To this day, fungi remain an important source of drugs for infectious diseases. With the rapid development of genome sequencing technology and the exploration of biosynthetic gene clusters, more novel compounds from fungi have been discovered. Fungi can be isolated from soil, water, air, plants and other organisms. In particular, endophytic fungi produce secondary metabolites similar to those of their hosts. Fungal libraries with a high degree of biodiversity are important for both academic research and industry.

Polyphenolic Natural Product Library

Catalog No. L6100 — 640 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.



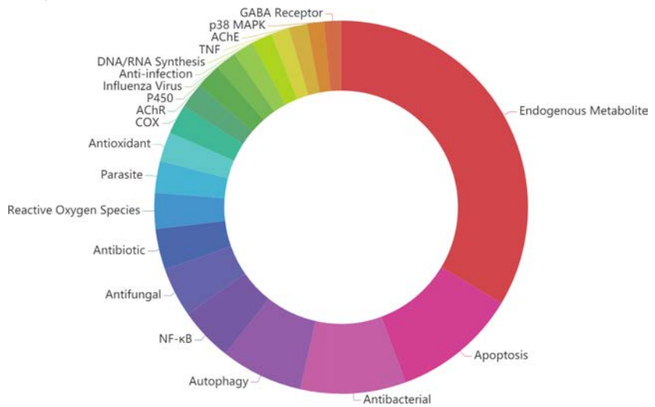
Natural Polyphenolic compound Library is a unique collection of 640 natural polyphenolic compounds, an effective tool for anti-cancer drug screening and high throughput screening (HTS) and high content screening (HCS).

RO5 Drug-like Natural Product Library

Catalog No. L6160 — 2,743 compounds

Natural products are important sources of lead compounds and drug candidates. They have complex scaffold structures and rich functional groups. Their structures are unique, and most of them are chiral. These naturally occurring advantages provide more diverse options for the transformation of natural products into drugs, and are also the reasons why natural products play an important role in drug development and research.

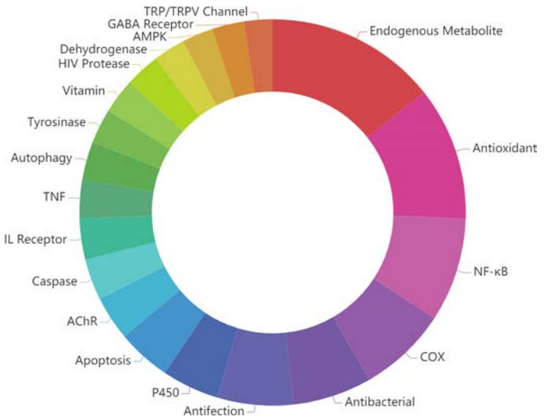
Based on the structural diversity and novelty of natural products, TargetMol used the druglikeness prediction index "Lipinski's Rule of Five" to select 2743 natural product monomers with good druggabilities, covering diverse structures from vast sources such as terpenes and alkaloids. The library is consisted of monomers with both biological activity and drug-like properties. It is a powerful tool for subsequent structure-effect optimization and innovative drug research.



Food as Medicine Compound Library

Catalog No. L6300 — 1,302 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. There are 101 substances included in the "Administrative Measures on the Catalogue of Substances Traditionally Considered as Both Food and Chinese Medicine" released by the National Health and Family Planning Commission (NHFPC) of China so far.

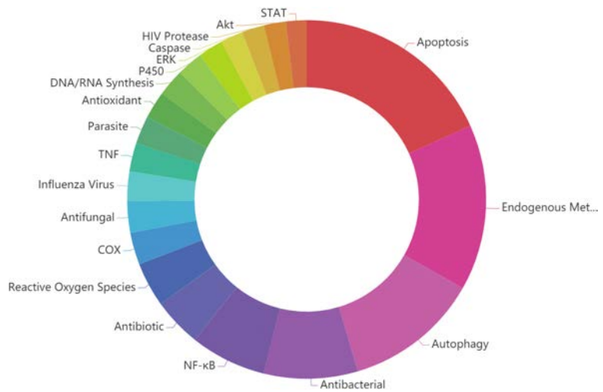


Based on the food as medicine raw materials published by NHFPC and related literature, TargetMol carefully collects 1302 compounds with safety guaranteed as Food as Medicine Compound Library, which can be used for high throughput and high content screening for drug discovery.

Anti-Tumor Natural Product Library

Catalog No. L6700 — 1,800 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 year 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.

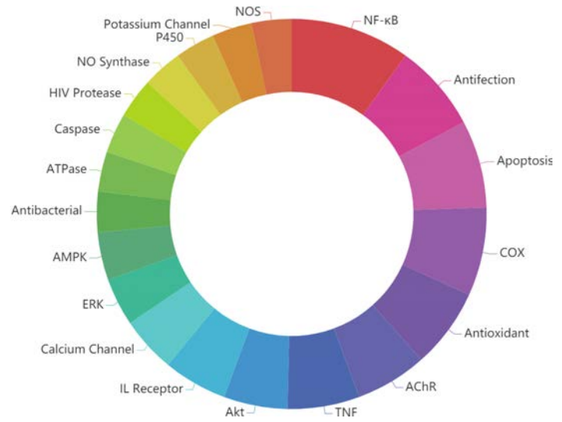


TargetMol carefully collects 1800 natural products from plants, animals, or microbes with known or potential antitumor activity, which is a powerful tool for your antitumor drug development and lead compounds screening.

Rare Natural Product Library

Catalog No. L6900 — 180 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 a privileged tools for the study and manipulation of protein function.



The TargetMol's Rare Natural Product Library, a unique collection of 180 rare natural products with known bioactivity and wide source, is a powerful tool for drug discovery, pharmacological study, and stem cell differentiation, etc.

Natural Product Libraries for CADD

Selectable Natural Product Library
Catalog No. L6020 — 16,627 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 from Artemisia annua and 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 16627 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.

Natural Product Derivatives Library for CADD
Catalog No. L6030 — 163,000 compounds

Natural products have been used in the treatment of disease since ancient times and have been the inspiration for modern drug discovery and development. In the past few decades, approximately 40% of FDA-approved marketed drugs have been natural products, natural product derivatives, or synthetic analogues related to natural products. Molecular scaffolds identified in natural products have significant structural diversity and drug-like properties, which can be used as a basis for designing structurally novel natural product derivatives.

With the development of high-throughput screening and virtual screening technologies, a large number of compounds can be analyzed for activity in a short period of time. However, due to difficulties in extraction and synthesis, natural products are usually limited in amounts, thus unable to go through screening studies as drug-like compounds. This problem has greatly hindered the development of natural product-related drugs.

Through combinatorial chemistry, a large number of derivatives and analogues can be synthesized using natural products as templates. Natural product derivatives can modify the intermediate structure while preserving the parent structure of the natural product, and by introducing different substituents, the loss of activity caused by the change of the parent structure can be avoided. Based on these advantages, natural product derivatives are more suitable for high-throughput screening and virtual screening.

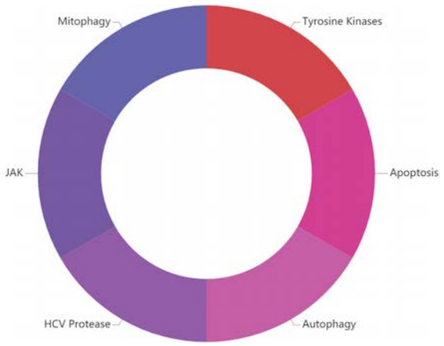
Because of the great interest of our customers in the research of natural product derivatives, TargetMol® has carefully compiled the structure data of more than 163,000 natural product derivatives and provided them to our customers free of charge. all the structures included in the database have corresponding compounds supplied by TargetMol® that can be purchased for subsequent research studies. What's more, there is always a library customization service for our customers to design their own product derivative library.

General Fragment Libraries

Featured Fragment Library
Catalog No. L5700 — 246 compounds

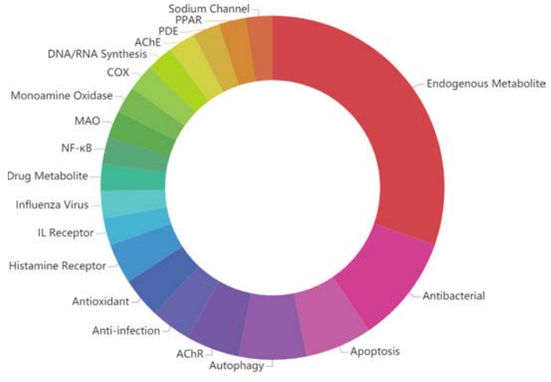
Fragment-based drug discovery (FBDD) has emerged in the past decade as a powerful tool for discovering drug leads. FBDD has played a role in discovery of at least 30 drugs that are in various stages of clinical development, and practitioners of FBDD can be found throughout the world in both academia 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.



High Solubility Fragment Library
Catalog No. L7800 — 2,731 compounds

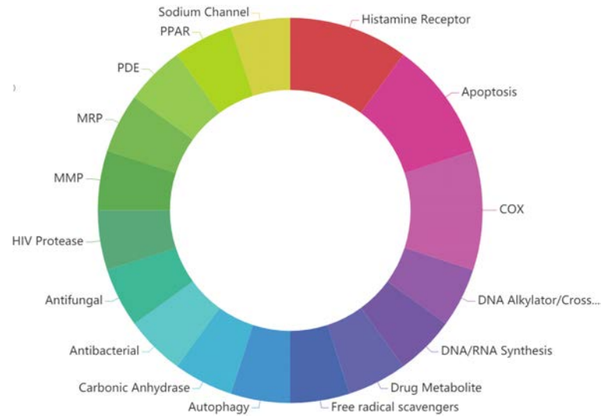
The TargetMol's Fragment Library Plus collects 2731 fragment-like small molecules meeting with strict Astex Rule of Three Criteria (MW ≤ 300, cLogP ≤ 3, H-bond donors ≤ 3 H-bond acceptors ≤ 3) for fragment based drug discovery.



Characteristic Fragment Libraries

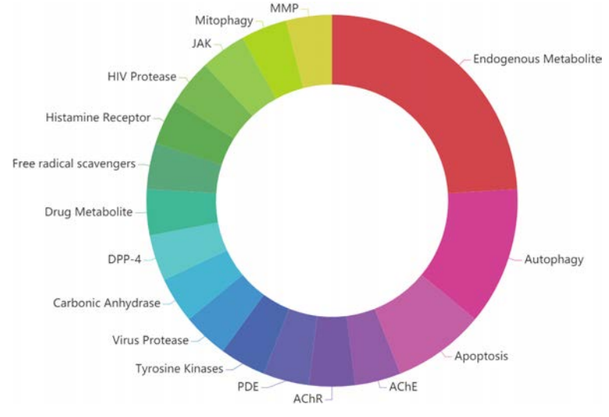
High Solubility Polyfunctional Group Fragment Library
Catalog No. L7810 — 1,159 compounds

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.



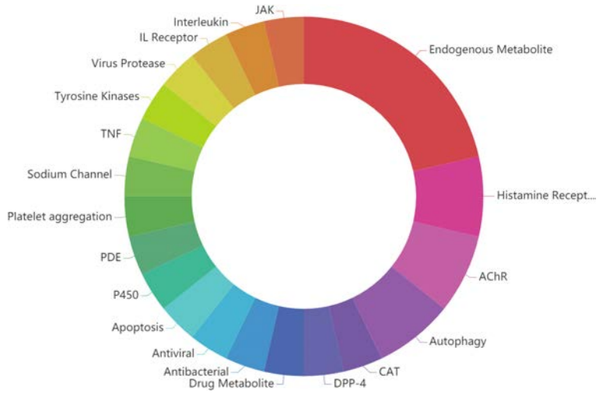
High Solubility Micro Fragment Library
Catalog No. L7820 — 1,082 compounds

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.



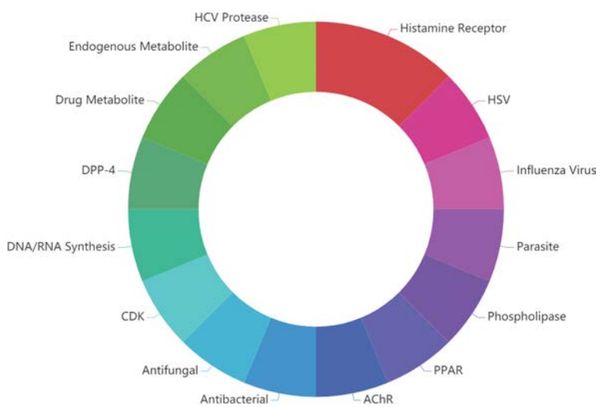
High Solubility Pharmacophore Fragment Library
Catalog No. L7830 — 985 compounds

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.



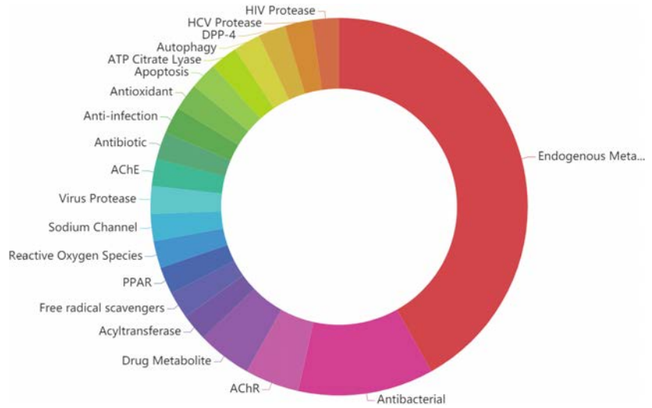
High Solubility FragLite Fragment Library
Catalog No. L7840 — 796 compounds

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.



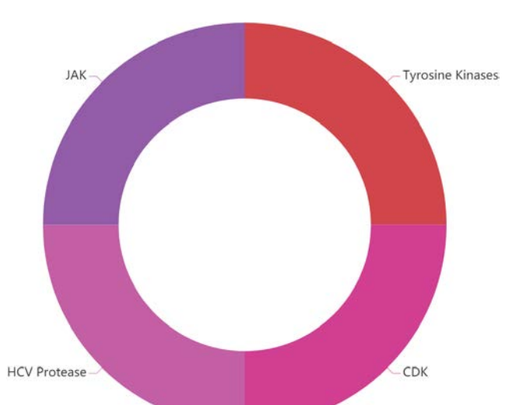
High Solubility 3D Diversity Fragment Library
Catalog No. L7850 — 1,081 compounds

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 1081 compounds.



Mini Electrophilic Heterocyclic Fragment Library
Catalog No. L7860 — 369 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. 369 compounds in total in the Highly Solubility Covalent Heterocyclic Fragment Library

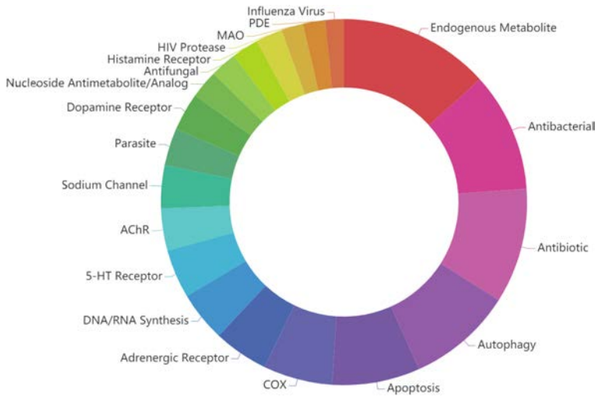


Drug-Fragment Library

Catalog No. L8800 — 1,158 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 1158 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.

Drug-like Diversity Compound Library

Mini Scaffold Library

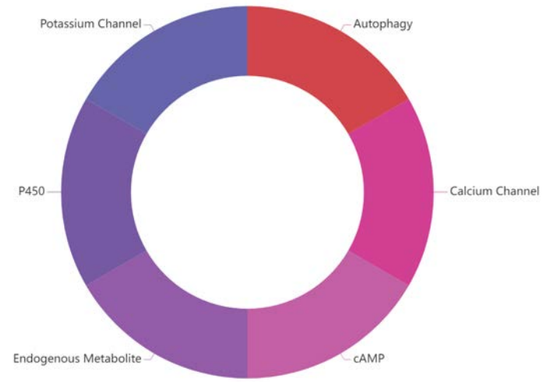
Catalog No. L5600 — 5,000 compounds

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 5000 compounds, representing 5000 scaffolds, from a large drug-like chemical source.

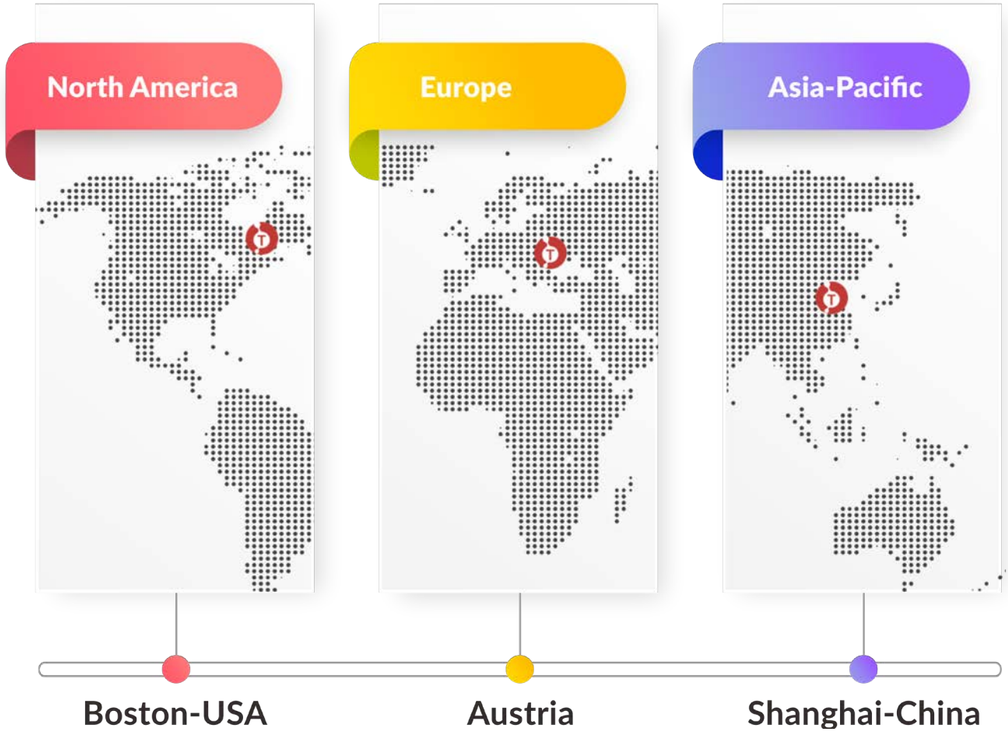
Golden Scaffold Library

Catalog No. L5610 — 10,000 compounds

While sourcing from 1,600,000 drug-like compounds, TargetMol's Golden Scaffolds Library of 10000 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.



Global Sites



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