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YOUR TARGET MOLECULES

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DRUG REPURPOSING

INHIBITORS & AGONISTS

COMPOUND LIBRARIES

RECOMBINANT PROTEINS

NATURAL PRODUCTS

TECHNICAL SERVICE

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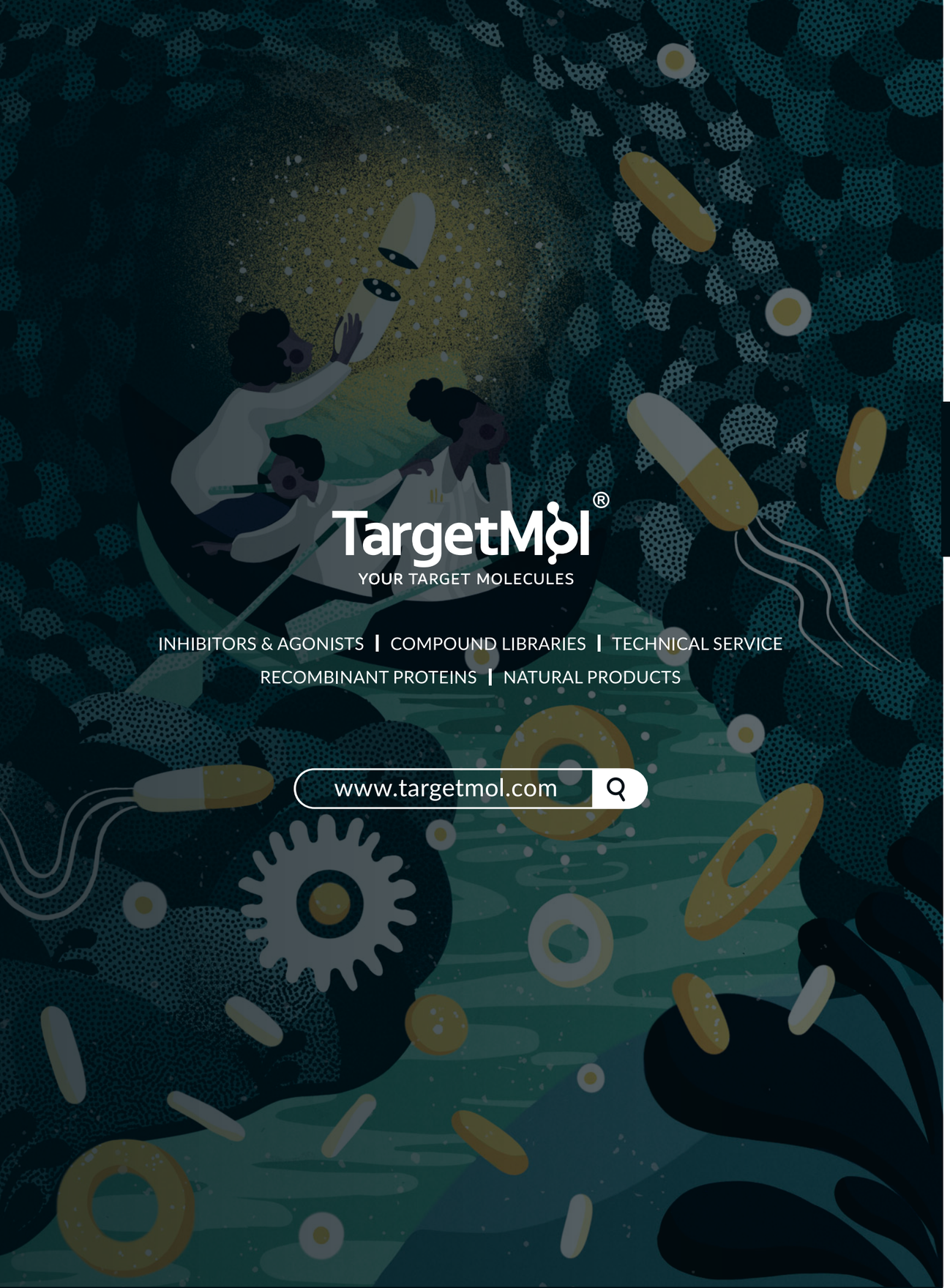

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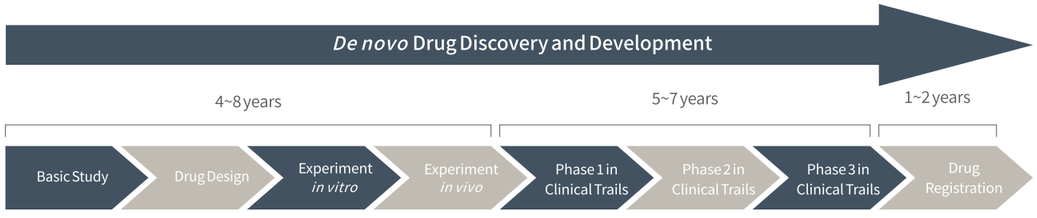
CONTENTS

Drug Repurposing

Drug repurposing is a strategy used to discover new therapeutic uses for existing drugs or investigational compounds beyond their originally approved indications. Drug repurposing offers the advantages of lower R&D costs and shorter development timelines, making it a promising approach for treating both common and rare diseases.

For example, Disulfiram, a medication that has been approved by FDA for over 60 years as a treatment for alcohol dependence. Recent studies have confirmed its potent anti-tumor properties, such as: inhibition of cancer stem cells, induction of tumor cell apoptosis, inhibition of proteasomes, induction of cell cycle arrest, inhibition of tumor angiogenesis, enhancing radiosensitivity, reversal of tumor cell drug resistance.

Metformin is originally a major medication used for the treatment of type 2 diabetes. Studies have found that, in addition to its glucose-lowering effects, it also has therapeutic effects on cardiovascular diseases, anti-tumor properties, anti-infection effects, anti-inflammatory effects, and anti-aging effects.



De novo Drug Discovery and Development:
- Low Success Rate
- Huge Cost and Time-consuming Development

Drug Repurposing:
- Known Drug Safety
- Reduced Pharmacokinetic Uncertainty

Drug Repurposing

Advantages of Drug Repurposing

01 **Lower Risk of Failure:** If the drug has completed early trials, it is proven to be safe in clinical models and humans. The risk of failure in subsequent efficacy trials is reduced.

02 **Shorter R&D Time:** It generally takes 13 to 15 years to bring a new drug to market. However, the development cycle for drug repurposing is significantly reduced because most of the preclinical testing, safety assessments, and formulation development have already been completed.

03 **Lower Investment Required:** Drug repurposing can help save a significant amount of costs in the preclinical, Phase I, and Phase II stages.

TargetMol's Advantages

An Extensive Range of Products

TargetMol provides an extensive range of products, including 50,000+ active small molecules, peptides, antibody inhibitors, dyes and reagents, PROTACs, recombinant proteins, and commonly used cell assay kits. Additionally, we offer 800+ compound libraries to meet diverse research needs.

Comprehensive Information and Data

Supported by a wealth of literatures and databases, our compounds (and libraries) are enriched with detailed biological and structural information.

High Quality Assurance

TargetMol adheres to high standards of quality control. NMR, HPLC, and LCMS. This guarantees that the compounds provided are of high purity and quality.

Professional Service

Our experienced technical team offers comprehensive and professional support.

WINNER

TARGETMOL

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Related Compounds

Aspirin, also known as acetylsalicylic acid, originates from the ancient practice of using willow bark in medicine. In the mid-19th century, acetylsalicylic acid was extracted from meadowsweet and introduced to the medical field. At the end of the 20th century, scientists discovered its anticoagulant mechanism, marking a significant breakthrough. Initially, aspirin was widely used as an antipyretic and analgesic for treating colds, headaches, and similar conditions. In 1950, it was found to potentially prevent myocardial infarction. In 1982, its mechanism of inhibiting platelet aggregation was discovered, a discovery that earned a Nobel Prize.

Catalog No.	Product Name	CAS	Application (Original)	Application (New)
T0005	Aspirin	50-78-2	Analgesic	Treatment of rheumatism and cardiovascular diseases
T0054	Disulfiram	97-77-8	Anti-Alcoholism Drugs	Anti cancer
T0213	Thalidomide	50-35-1	Tranquilizer	Treatment of leprosy and multiple melanomas
T0968	Paclitaxel	33069-62-4	Phytochemicals with Anti-Cancer Properties	Anti-coronary artery stenosis; Anti-liver/kidney tissue fibrosis
T1537	Rapamycin	53123-88-9	Immunosuppressant	Treatment of lymphangioleiomyomatosis (LAM)
T4006	Pentostatin	53910-25-1	Leukemia Treatment	Treatment agent for hairy cell leukemia
T8526	Metformin	657-24-9	Diabetes Treatment	Anti cancer; Anti aging
T77798	Glypromate	32302-76-4	Antidote for Cyanide Poisoning	Treatment of sickle cell anemia and other blood diseases caused by chronic leg ulcers

Drug Repurposing Compound Library

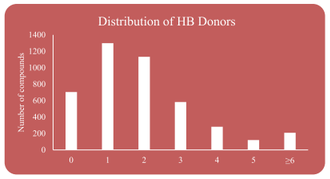
L9200

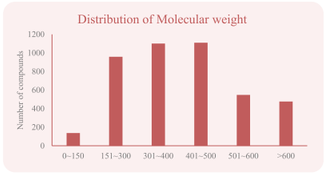
Traditional de novo drug discovery and development involves an HTS campaign for de novo candidate hits and requires highly specialized screening facilities and compound libraries containing several million compounds. It is a time consuming and expensive process. As the regulation for drug safety and 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.

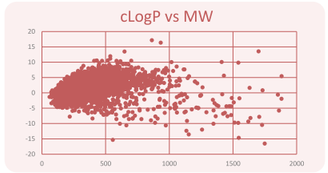
TargetMol's Drug Repurposing Compound Library, containing 4,900+ approved and clinical drugs, has undergone extensive preclinical studies and have well-characterized bioactivities, safety and bioavailability.

- A unique collection of 4,900+ approved and clinical drugs for high throughput screening (HTS) and high content screening (HCS);
- All approved drugs collected in this library are approved by Food and Drug Administration (FDA), the European Medicine Agency (EMA), or National Medical Products Administration (NMPA), or included in the US Pharmacopeia (USP) Dictionary, the British Pharmacopoeia (BP), the European Pharmacopoeia (EP), the Japanese Pharmacopoeia (JP), or Chinese Pharmacopoeia (CP) Dictionary;
- Covers various research areas, such as cancer, cardiovascular disease, immunology, respiratory system, etc.
- Covers various targets, such as 5-HT Receptor, Sodium Channel, p38 MAPK, PI3K, MEK, etc.
- Detailed compound information with structure, target, activity, and brief introduction;
- Structurally diverse, medicinally active, and cell permeable;
- NMR and HPLC validated to ensure high purity and quality.

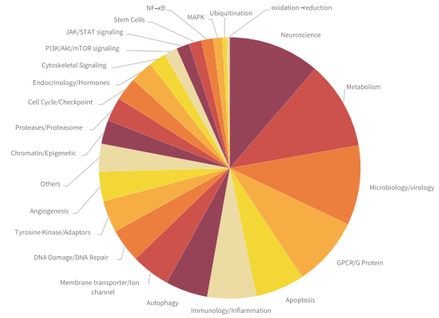
Compounds Compliant With Lipinski's Rules	
PhysChem Properties	% Compounds
Hbond donors <5	92%
HBond acceptors <10	93%
cLogP<5	88%
MW<500	76%



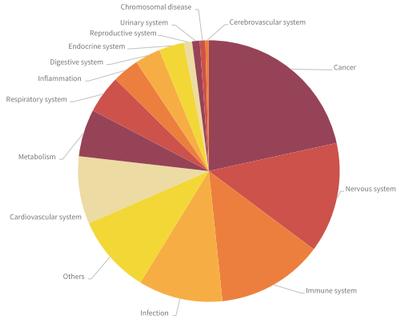




Analysis of Drug-Like Properties



Composition of Signaling Pathways



Related Research Fields

Related Compound Libraries

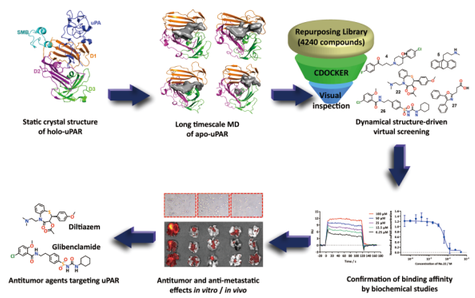
Catalog No.	Product Name	Quantity	Description
L4010	Bioactive Compounds Library Max	25,000+	A collection of 25,000+ bioactive compounds for high-throughput screening, high-content screening, cell induction and target identification.
L1000	Approved Drug Library	2,800+	A unique collection of 2,800+ approved drugs for high throughput screening and high content screening; All compounds are drugs approved by FDA, EMA, or NMPA, etc.
L4200	FDA-Approved Drug Library	1,800+	A unique collection of 1,800+ FDA approved drugs for high throughput screening and high content screening.
L1010	FDA-Approved & Pharmacopeia Drug Library Clinical Compound Library	3,100+	A collection of 3,100+ compounds for high throughput screening and high content screening; All compounds are drugs approved by FDA, EMA, PMDA, NMPA, etc. or included in pharmacopoeia such as USP, BP, JP, etc.
L3400	Preclinical Compound Library	3,400+	A unique collection of 3,400+ compounds in clinical trial phases for high throughput screening and high content screening; All compounds have been permitted into clinical trial phases, categorized into Phase 1, Phase 2 and Phase 3.

Application Cases

Journal of Medicinal Chemistry, 2023, 66(8): 5415-5426

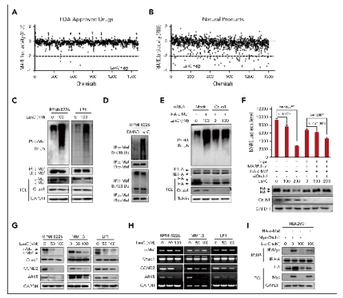
The author, targeting the urokinase receptor (uPAR), employed structure dynamics-driven virtual screening using the **TargetMol-L9200 Drug Repurposing Compound Library (containing 4,900+ compounds)**. Through this process, Diltiazem and Glibenclamide were identified as potential agents with anti-tumor and anti-metastatic activities.

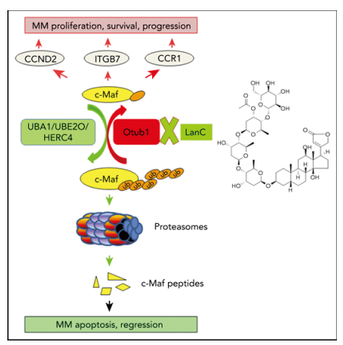
Virtual Screening of Small-Molecule Compounds Intervening with the uPA–uPAR Interaction. Based on the most representative structures of the four dominant clusters of apo-uPAR obtained from the above long-timescale MD simulation, we performed a multiple docking-based virtual screening against the TargetMol Drug Repurposing Compound Library L9200 (including 4,240 compounds, https://www.targetmol.com/all-compound-libraries) using the CDOCKER module implemented in Discovery Studio 2017 R2 Client. The consensus analysis was performed on seven different scoring functions (Figure S2A and see Additional Experimental Section in Supporting Information for details).



Blood, The Journal of the American Society of Hematology, 2021, 137(11): 1478-1490.

Previous research has identified the Otub1/c-Maf axis as a potential new therapeutic target for multiple myeloma (MM). In order to explore this concept, in the present study, the authors utilized the **L4200-FDA-Approved Drug Library and the L6000-Natural Product Library for HTS from Targetmol** to perform a screen. From this screening, the generic cardiac glycoside lanatoside C (LanC) is found to prevent c-Maf deubiquitination and induces its degradation by disrupting the interaction of Otub1 and c-Maf. Consequently, LanC inhibits c-Maf transcriptional activity, induces c-Maf-expressing MM cell apoptosis, and suppresses MM growth and prolongs overall survival of model mice, but without apparent toxicity. Therefore, the present study identifies Otub1 as a novel deubiquitinase of c-Maf and establishes that the Otub1/c-Maf axis is a potential therapeutic target for MM.

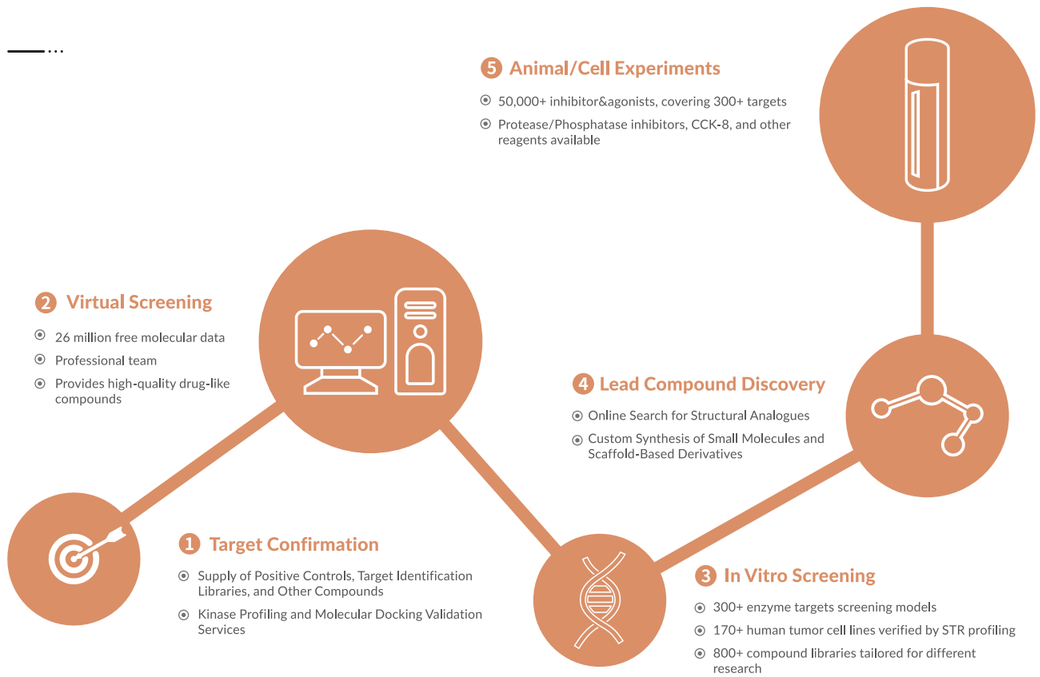




HEK293T cells co-transfected with the pMARE.Luci [10], c-Maf and Otub1 plasmids were incubated with each compound (5 μM) from TargetMol® collections of FDA-approved drugs and natural products. Luciferase activity was analyzed with the Bright-Glo substrate (Promega) as described previously [8]. The detailed screen was described in Supplemental Methods.

Catalog No.	Product Name	Quantity	Description
L3410	Preclinical Compound Library	700+	Preclinical Compound Library is a collection of 700+ compounds that are in preclinical phase with clear targets and detailed information on disease indication and reference.
L4000	Bioactive Compound Library	17,000+	A collection of 17,000+ small molecule compounds with validated activity for high throughput screening, high content screening, cell induction, and target identification.
L2110	Anti-Cancer Approved Drug Library	1,700+	TargetMol selects 1,700+ approved anti-cancer drugs based on published literatures and database to form this collection that can be used as positive controls in biological cancer investigation and cancer correlation study.
L1610	FDA-Approved Kinase Inhibitor Library	260+	Targetmol's FDA-Approved Kinase Inhibitor Library contains 280 marketed drugs that target kinases. These kinases include Insulin/IGF Receptors、PI 3-Kinase、CaM Kinase II、JAK、PKA、CDK、JNK、PKC、CKI II、MAPK、RAF、EGFR、MEK、SAPK、GSK、MLCK、Src-family、IKK、PDGFR、VEGFR etc.
L1600	Kinase Inhibitor Library	2,800+	TargetMol's Kinase Inhibitor Library, containing 2,800+ kinase inhibitors/regulators , can be used for research in chemical genomics, pharmacological study, and drug screening for related diseases.
L2100	Anti-Cancer Compound Library	8,700+	TargetMol selects 8,700+ compounds with anti-tumor activity based on different characteristics and abnormal metabolism with cancer cells. These compounds are the small molecules modulating the metabolism, growth, invasion, and metastasis of tumor cells.
L1200	Epigenetics Compound Library	1,000+	TargetMol's Epigenetics Compound Library, containing 1090 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.

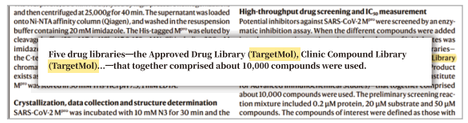
Technical Services



Citations (Part)

Nature. 2020 Jun;582(7811):289-293.

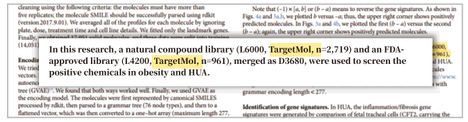
Structure of Mpro from COVID-19 virus and discovery of its inhibitors



Five drug libraries—the Approved Drug Library (TargetMol), Clinic Compound Library (TargetMol)...—that together comprised about 10,000 compounds were used.

Nat Biotechnol. 2021 Nov;39(11):1444-1452.

Prediction of drug efficacy from transcriptional profiles with deep learning



In this research, a natural compound library (L6000, TargetMol, n=2,719) and an FDA-approved library (L4200, TargetMol, n=961), merged as D3680, were used to screen the positive chemicals in obesity and HUA.

Nat Genet. 2018 Dec;50(12):1666-1673.

Cilia-driven cerebrospinal fluid flow directs expression of urotensin neuropeptides to straighten the vertebrate body axis

The GPCR compound library was purchased from Target Molecule Corporation, and contains 356 active compounds that target G proteins and GPCRs.

Cancer Cell. 2019 Jan 14;35(1):125-139.e9.

The ERBB-STAT3 axis drives Tasmanian devil facial tumor disease

Blood. 2021 Mar 18;137(11):1478-1490.

Targeting the Otub1/c-Maf axis for the treatment of multiple myeloma

Nucleic Acids Res. 2021 Sep 7;49(15):8974-8986.

Small-molecule compounds boost genome-editing efficiency of cytosine base editor

Angew Chem Int Ed Engl. 2022 Jan 17;61(3):e202113515.

Multiplexed Small-Molecule-Ligand Binding Assays by Affinity Labeling and DNA Sequence Analysis

- Nature. 2020, 582: 289-293 —— Approved Drug Library;Clinical Compound Library
- Nature Biotechnology. 2021, 39(11): 1444-1452 —— FDA Approved Drug Library;Natural Product Library for HTS
- ACS Central Science. 2023, 9(10): 1927-1943. —— FDA Approved Drug Library
- Nature Communications. 2023, 14(1): 1020. —— FDA Approved Drug Library;Traditional Chinese Medicine Monomer Library
- Nature Communications. 2023, 14(1): 2756. —— FDA Approved Drug Library
- Blood. 2021, 137(11): 1478-1490 —— FDA Approved Drug Library;Natural Product Library for HTS
- Nucleic Acids Research. 2021, 49(15): 8974-8986. —— Approved Drug Library
- Advanced Science. 2021, 8(18): 2101957. —— FDA Approved Drug Library
- Nature Communications. 2023, 14(1): 7574 —— Approved Drug Library;Clinical Compound Library
- Protein & Cell. 2021, 12(11): 877-888 —— Approved Drug Library;Clinical Compound Library
- Protein & Cell. 2021, 12(10): 769-787. —— FDA Approved Drug Library
- Bone Research. 2023, 11(1): 54 —— FDA Approved Drug Library;Natural Product Library for HTS

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