

# DRUG REPURPOSING



INHIBITORS &  
AGONISTS



COMPOUND  
LIBRARIES



RECOMBINANT  
PROTEINS



NATURAL  
PRODUCTS



TECHNICAL  
SERVICE

Distributed by:

**CliniSciences Group**





INHIBITORS & AGONISTS | COMPOUND LIBRARIES | TECHNICAL SERVICE  
RECOMBINANT PROTEINS | NATURAL PRODUCTS

## CONTENTS

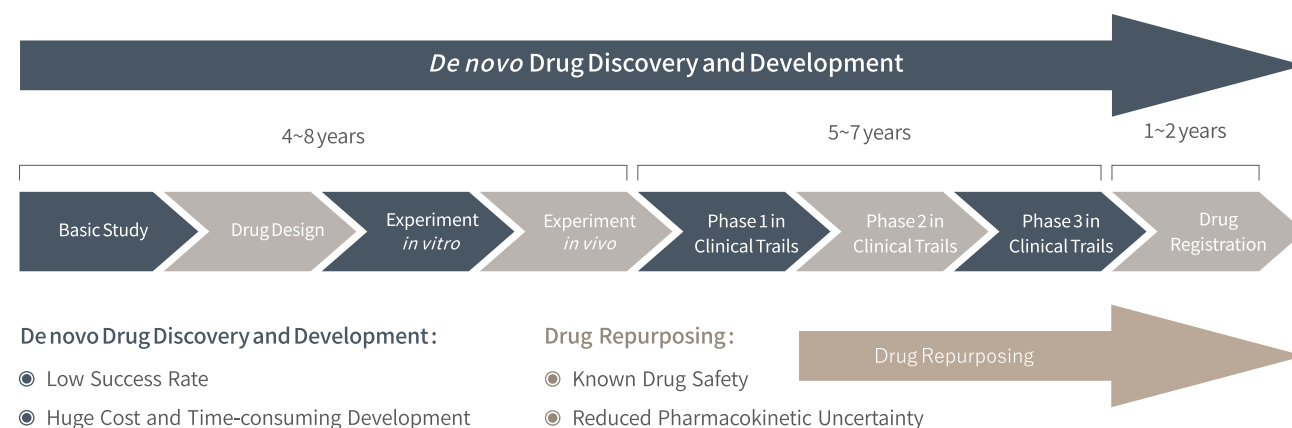
|                                   |    |
|-----------------------------------|----|
| Drug Repurposing                  | 01 |
| Advantages of Drug Repurposing    | 01 |
| TargetMol's Advantages            | 02 |
| Related Compounds                 | 02 |
| Drug Repurposing Compound Library | 03 |
| Related Compound Libraries        | 04 |
| Technical Services                | 05 |
| Application Cases                 | 06 |
| Citations (Part)                  | 07 |

# 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.



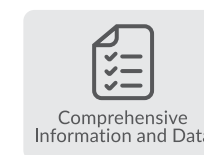
# Advantages of Drug Repurposing

- 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



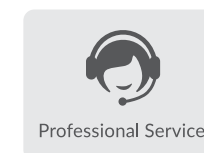
TargetMol provides an extensive range of products, including 50,000+ active small molecules, peptides, antibody inhibitors, dyes and reagents, PROTACs, recombinant proteins, and commonly used cell assay kits. Additionally, we offer 800+ compound libraries to meet diverse research needs.



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



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



Our experienced technical team offers comprehensive and professional support.



WINNER

**TARGETMOL**

BIOCHEMICAL SUPPLIER TO WATCH IN 2023



**CiteAb**



# 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.

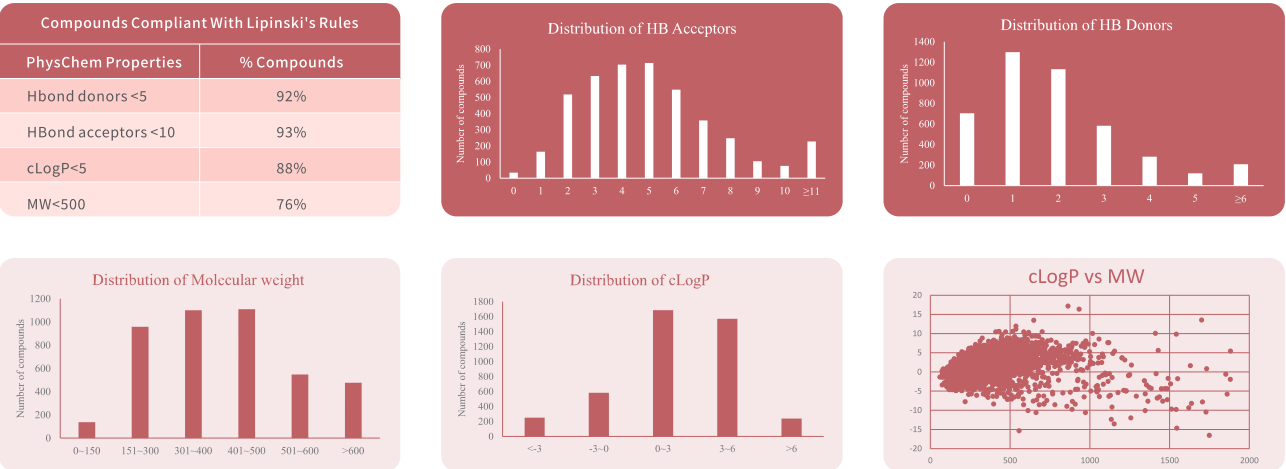
| Catalog No. | Product Name | CAS        | Application (Original)                     | Application (New)                                                                     |
|-------------|--------------|------------|--------------------------------------------|---------------------------------------------------------------------------------------|
| 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

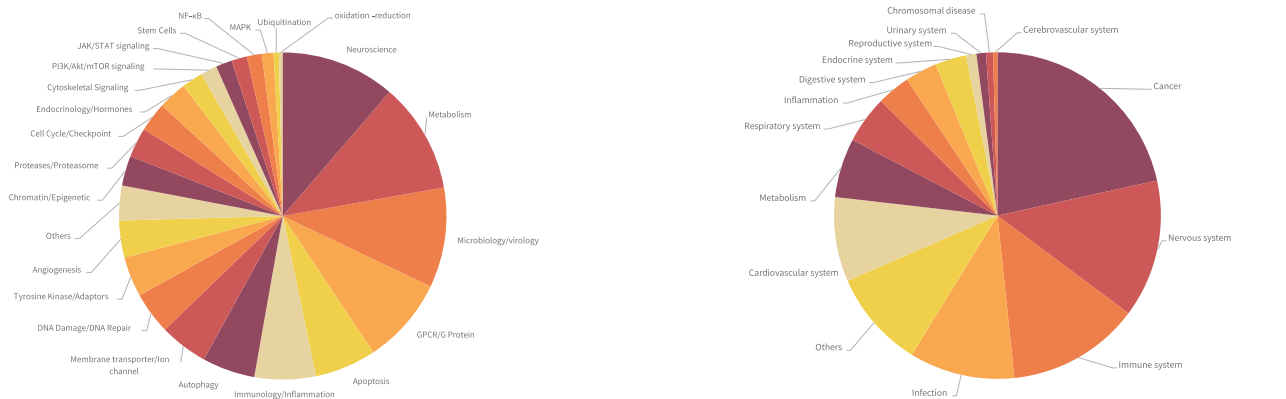
Traditional de novo drug discovery and development involves an HTS campaign for de novo candidate hits and requires highly specialized screening facilities and compound libraries containing several million compounds. It is a time consuming and expensive process. As the regulation for drug safety and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



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. |

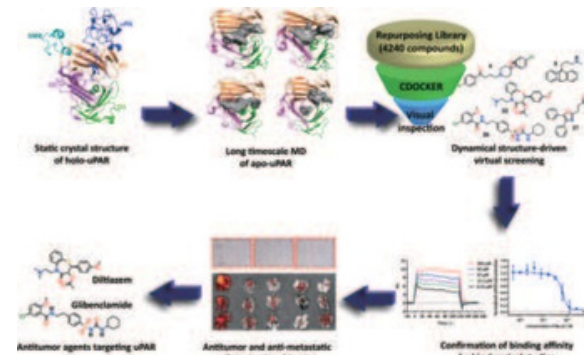


# Application Cases

## 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.

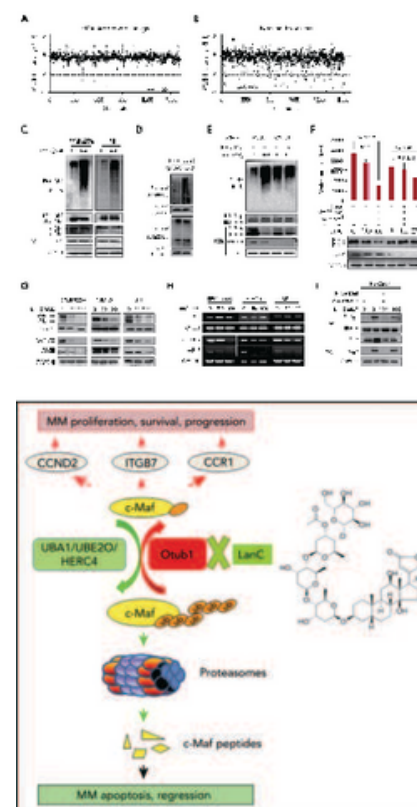
**Virtual Screening of Small-Molecule Compounds Intervening with the uPA-uPAR Interaction.** Based on the most representative structures of the four dominant clusters of apo-uPAR obtained from the above long-timescale MD simulation, we performed a multiple docking-based virtual screening against the **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.

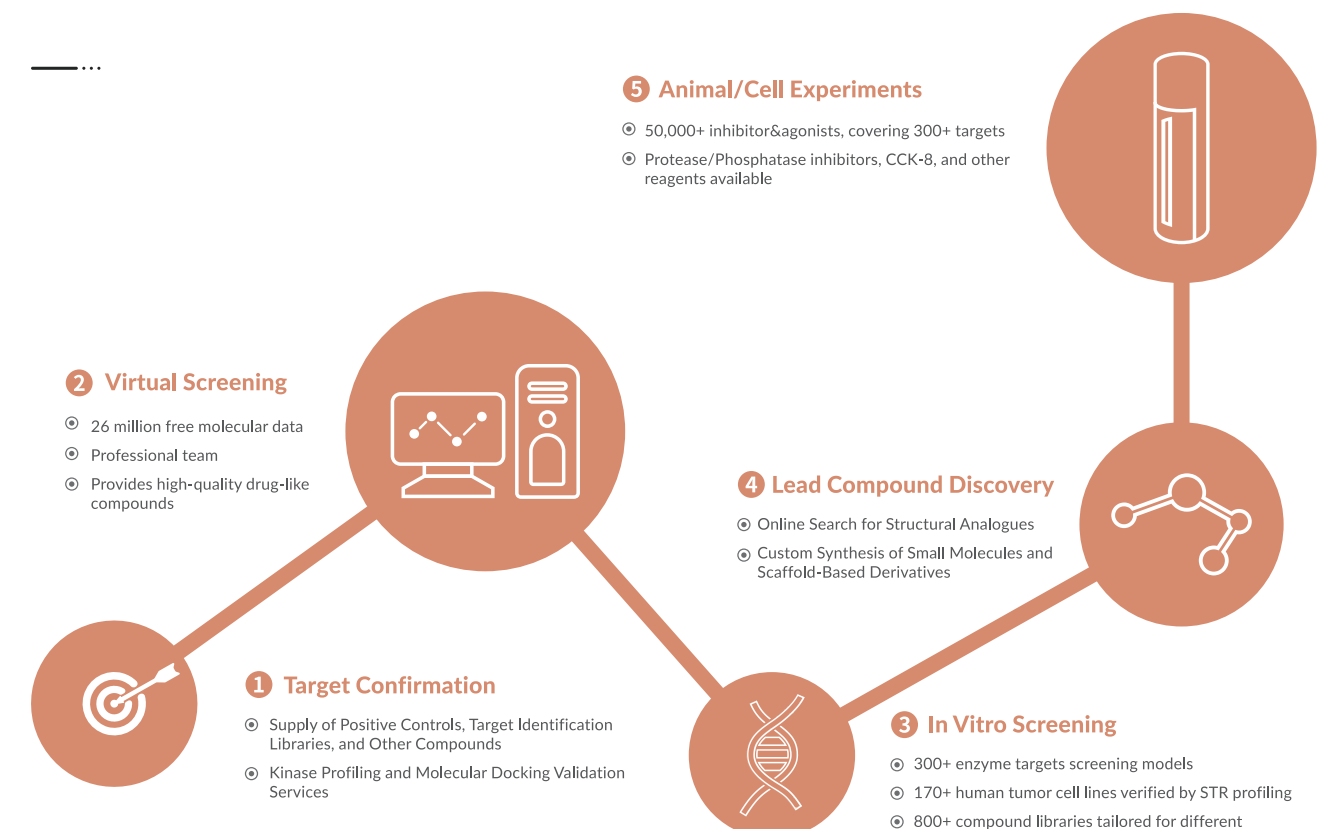
Previous research has identified the Otub1/c-Maf axis as a potential new therapeutic target for multiple myeloma (MM). In order to explore this concept, in the present study, the authors utilized the **L4200-FDA-Approved Drug Library and the L6000-Natural Product Library for HTS from Targetmol** to perform 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<sup>30</sup>, c-Maf and Otub1 plasmids were incubated with each compound (5 μM) from TargetMol<sup>®</sup> collections of **FDA-approved drugs and natural products**. Luciferase activity was analyzed with the Bright-Glo substrate (Promega) as described previously<sup>8</sup>. 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



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

## Prediction of drug efficacy from transcriptional profiles with deep learning



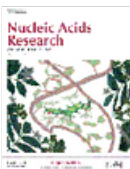
**Nat Genet.** 2018 Dec;50(12):1666-1673.

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



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

## The ERBB-STAT3 axis drives Tasmanian devil facial tumor disease



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

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



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

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



**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









# CliniSciences Group

## Austria

Company: CliniSciences GmbH  
Address: Sternwartestrasse 76, A-1180  
Wien - Austria  
Telephone: +43 720 115 580  
Fax: +43 720 115 577  
Email: [oesterreich@clinisciences.com](mailto:oesterreich@clinisciences.com)  
Web: <https://www.clinisciences.com>



## Belgium

Company: CliniSciences S.R.L.  
Address: Avenue Stalingrad 52, 1000  
Brussels - Belgium  
Telephone: +32 2 31 50 800  
Fax: +32 2 31 50 801  
Email: [belgium@clinisciences.com](mailto:belgium@clinisciences.com)  
Web: <https://www.clinisciences.com>



## Denmark

Company: CliniSciences ApS  
Address: Oesterbrogade 226, st. 1,  
Copenhagen, 2100 - Denmark  
Telephone: +45 89 888 349  
Fax: +45 89 884 064  
Email: [denmark@clinisciences.com](mailto:denmark@clinisciences.com)  
Web: <https://www.clinisciences.com>



## Finland

Company: CliniSciences ApS  
Address: Oesterbrogade 226, st. 1,  
Copenhagen, 2100 - Denmark  
Telephone: +45 89 888 349  
Fax: +45 89 884 064  
Email: [suomi@clinisciences.com](mailto:suomi@clinisciences.com)  
Web: <https://www.clinisciences.com>



## France

Company: CliniSciences S.A.S  
Address: 74 Rue des Suisses, 92000  
Nanterre- France  
Telephone: +33 9 77 40 09 09  
Fax: +33 9 77 40 10 11  
Email: [info@clinisciences.com](mailto:info@clinisciences.com)  
Web: <https://www.clinisciences.com>



## Germany

Company: Biotrend Chemikalien GmbH  
Address: Wilhelm-Mauser-Str. 41-43,  
50827 Köln - Germany  
Telephone: +49 221 9498 320  
Fax: +49 221 9498 325  
Email: [info@biotrend.com](mailto:info@biotrend.com)  
Web: <https://www.biotrend.com>



## Iceland

Company: CliniSciences ApS  
Address: Oesterbrogade 226, st. 1,  
Copenhagen, 2100 - Denmark  
Telephone: +45 89 888 349  
Fax: +45 89 884 064  
Email: [island@clinisciences.com](mailto:island@clinisciences.com)  
Web: <https://www.clinisciences.com>



## Ireland

Company: CliniSciences Limited  
Address: Ground Floor, 71 lower Baggot street  
Dublin D02 P593 - Ireland  
Telephone: +353 1 6971 146  
Fax: +353 1 6971 147  
Email: [ireland@clinisciences.com](mailto:ireland@clinisciences.com)  
Web: <https://www.clinisciences.com>



## Italy

Company: CliniSciences S.r.l  
Address: Via Maremmana inferiore 378  
Roma 00012 Guidonia Montecelio - Italy  
Telephone: +39 06 94 80 56 71  
Fax: +39 06 94 80 00 21  
Email: [italia@clinisciences.com](mailto:italia@clinisciences.com)  
Web: <https://www.clinisciences.com>



## Netherlands

Company: CliniSciences B.V.  
Address: Kraijenhoffstraat 137A,  
1018RG Amsterdam, - Netherlands  
Telephone: +31 85 2082 351  
Fax: +31 85 2082 353  
Email: [nederland@clinisciences.com](mailto:nederland@clinisciences.com)  
Web: <https://www.clinisciences.com>



## Norway

Company: CliniSciences AS  
Address: c/o MerVerdi Munkerudtunet 10  
1164 Oslo - Norway  
Telephone: +47 21 988 882  
Email: [norge@clinisciences.com](mailto:norge@clinisciences.com)  
Web: <https://www.clinisciences.com>



## Poland

Company: CliniSciences sp.Z.o.o.  
Address: ul. Rotmistrza Witolda Pileckiego 67  
lok. 200 - 02-781 Warszawa -Poland  
Telephone: +48 22 307 0535  
Fax: +48 22 307 0532  
Email: [polska@clinisciences.com](mailto:polska@clinisciences.com)  
Web: <https://www.clinisciences.com>



## Portugal

Company: Quimigen Unipessoal LDA  
Address: Rua Almada Negreiros, Lote 5, Loja 14,  
2615-275 Alverca Do Ribatejo - Portugal  
Telephone: +351 30 8808 050  
Fax: +351 30 8808 052  
Email: [info@quimigen.com](mailto:info@quimigen.com)  
Web: <https://www.quimigen.pt>



## Spain

Company: CliniSciences Lab Solutions  
Address: C/ Hermanos del Moral 13  
(Bajo E), 28019, Madrid - Spain  
Telephone: +34 916 750 700  
Fax: +34 91 269 40 74  
Email: [espana@clinisciences.com](mailto:espana@clinisciences.com)  
Web: <https://www.clinisciences.com>



## Sweden

Company: CliniSciences ApS  
Address: Oesterbrogade 226, st. 1,  
Copenhagen, 2100 - Denmark  
Telephone: +45 89 888 349  
Fax: +45 89 884 064  
Email: [sverige@clinisciences.com](mailto:sverige@clinisciences.com)  
Web: <https://www.clinisciences.com>



## Switzerland

Company: CliniSciences AG  
Address: Fracht Ost Flughafen Kloten  
CH-8058 Zürich - Switzerland  
Telephone: +41 (044) 805 76 81  
Fax: +41 (044) 805 76 75  
Email: [switzerland@clinisciences.com](mailto:switzerland@clinisciences.com)  
Web: <https://www.clinisciences.com>



## UK

Company: CliniSciences Limited  
Address: 11 Progress Business center, Whittle  
Parkway, SL1 6DQ Slough- United Kingdom  
Telephone: +44 (0)1753 866 511  
or +44 (0) 330 684 0982  
Fax: +44 (0)1753 208 899  
Email: [uk@clinisciences.com](mailto:uk@clinisciences.com)  
Web: <https://www.clinisciences.com>



## USA

Company: CliniSciences LLC  
Address: c/o Carr Riggs Ingram,  
500 Grand Boulevard, Suite 210 Miramar  
Beach, FL 32550- USA  
Telephone: +1 850 650 7790  
Fax: +1 850 650 4383  
Email: [usa@clinisciences.com](mailto:usa@clinisciences.com)  
Web: <https://www.clinisciences.com>

