MCE®
MedChemExpress

ONE-STOP
COMPOUND SCREENING PLATFORM

MedChemExpress compound screening service, combined with **MedChemExpress** Bioactive Compound Libraries, Diversity Libraries, and Fragment Libraries, provides a 'One-Stop Compound Screening Platform' for customers working on drug discovery, target discovery and validation, and other basic and translational research projects.

ONE-STOP COMPOUND SCREENING PLATFORM

MedChemExpress one-stop compound screening platform supplies more than 200 screening libraries and a variety of compounds and phenotypic screening services. These services include DNA-encoded compound library screening, virtual screening, high-throughput screening (HTS), ion channel detection, kinase screening & profiling, phenotypic screening, affinity mass spectrometry screening, customized compound synthesis, structural optimization and analysis services, etc.

We are committed to continuously developing and improving our platform capabilities. Our goal is to creat a one-stop drug discovery service platform suitable for scientific research, and fostering infinite possibilities for innovation.

01

COMPOUND SCREENING LIBRARIES

- Bioactive Compound Libraries (BCL)
- Diversity Compound Libraries (DCL)
- High-Throughput Screening Libraries (HTSL)
- Fragment Libraries (FL)
- DNA-Encoded Compound Libraries (DEL)

02

VIRTUAL SCREENING

- Professional Drug Design Team
- 26 Million+ Compounds
- 2D/3D Molecular Docking Representation (SCI)

03

SCREENING SERVICES

- Drug Screening Services
- Stable and Efficient AS-MS Screening
- 30+ Ion Channel Stable Cell Lines
- 100+ GPCR Stable Cell Lines
- 400+ Kinase Profiles
- 120+ Tumor Cell Lines
- DEL Screening

04

LEAD COMPOUND OPTIMIZATION

- Search and Supply of Structure Analogs
- Custom Synthesis
- Analytical Development & Quality Control

TOP PUBLICATIONS CITING USE OF MEDCHEMEXPRESS PRODUCTS

Nature. 2023 Apr;616(7957):563-573.

Nature. 2023 Apr;616(7956):348-356.

Nature. 2023 Apr;616(7956):357-364.

Nature. 2023 Apr;616(7958):806-813.

Nature. 2023 Mar;615(7952):490-498.

Nature. 2023 Mar;615(7952):526-534.

Nature. 2023 Mar;615(7951):349-357.

Nature. 2023 Mar;615(7950):127-133.

Nature. 2023 Mar;615(7950):158-167.

Nature. 2023 Feb;614(7947):326-333.

Nature. 2023 Jan;613(7942):187-194.

Nature. 2023 Jan;613(7942):120-129.

Nature. 2022 Dec;612(7941):725-731.

Science. 2022 Dec 2;378(6623):eabo5503.

Science. 2022 Nov 18;378(6621):eabq7361.

Science. 2022 Oct 14;378(6616):eabq0132.

Science. 2022 Jul 8;377(6602):eabg9302.

Science. 2022 Mar 18;375(6586):1254-1261.

Cell. 2023 Apr 27;186(9):1895-1911.e21.

Cell. 2023 Mar 30;186(7):1352-1368.e18.

Cell. 2023 Mar 2;186(5):1026-1038.e20.

Cell. 2023 Feb 16;186(4):850-863.e16.

Cell. 2023 Feb 16;186(4):803-820.e25.

Cell. 2023 Feb 2;186(3):591-606.e23.

Cell. 2023 Jan 19;186(2):346-362.e17.

Cell. 2023 Jan 19;186(2):413-427.e17.

Cell. 2022 Nov 10;185(23):4347-4360.e17.

CONTENTS

Compound Screening Libraries

Virtual Screening

Drug Screening Services

Lead Compounds Optimization

COMPOUND SCREENING LIBRARIES

DIVERSE PRODUCT CATEGORIES

- 20, 000+ bioactive compounds
- 26 million+ diversity compounds and fragments
- 2 billion DEL molecules

RICH EXPERIENCE

- With more than 10 years of excellent experience in compound synthesis and compound library design
- >8,000 m² R&D center square, 1,000+ R&D staff
- Serving hundreds of thousands of scientists in more than 50 countries around the world
- Total deliveries exceeded 500,000 tubes of compounds

FULL PROCESS SERVICES

We provide the full-process drug development services covering compound library supply, screening services, lead compound optimization, and customized synthesis of compounds for preclinical and clinical studies

STRICT QUALITY MANAGEMENT SYSTEM

- Certified by ISO 9001, CNAS quality management system, strict quality control and verification system
- Since 2018, we have successfully cleared over 100 customer audits, with a flawless pass rate of 100%, and 11 third-party audits, including a GMP audit of EU QP
- Equipped with hundreds of state-of-the-art quality inspection equipment. Provide various quality inspection reports, including HNMR, LC/MS, HPLC, chiral analysis, elemental analysis, SEC-HPLC, etc

ADVANCED COMPOUND MANAGEMENT SYSTEM

- Have a global network of multiple business and warehouse logistics centers, sufficient spot reserves, stable supply chains
- 1,000 m^2 warehouse, stores over 100,000 sample tubes
- Fully automatic storage and selection of samples
- Fully airtight dry gas protection environment from room temperature to -80 °C

BIOACTIVE COMPOUND LIBRARY

- 200+ bioactive compound libraries
- 22,000+ bioactive compounds can be supplied
- Covering 1,000+ targets and hot research areas

FRAGMENT LIBRARY

- 20,000+ fragment compounds
- Diverse structures
- A useful tool for fragment-based drug discoveries (FBDD)

DIVERSITY COMPOUND LIBRARY

- 100,000+ compounds with highly diverse chemical structures
- Lead-like compounds with excellent bioactivity and high target-binding capacities
- The reliable and rich source for drug screening

HIGH-THROUGHPUT SCREENING LIBRARY

- 26 million+ compounds available for screening
- Suitable for AI-based lead discovery, ultra-large virtual screening
- Diverse and lead-like

DNA-ENCODED COMPOUND LIBRARIES

- 68 DEL libraries with billions of DEL molecules
- Highly diverse structures, wide chemical space coverage, high target-binding capacities
- Powerful compound synthesis capability
- Customized services

Compound Screening Libraries

01. BIOACTIVE COMPOUND LIBRARIES

Bioactive compounds are a general term for a class of substances that can cause specific biological effects in the body, which are the primary source of small molecule drugs. These compounds act on specific target proteins in cell-regulate intracellular signaling pathways, and cause some changes in cell phenotype.

Library Recommendation

HY-L001P Bioactive Compound Library Plus

This library has a full range of bioactive compounds, including natural products, innovative compounds, approved compounds, and clinical compounds. This library is a valuable tool for signal pathway research, drug discovery, repurposing, etc.

HY-L099 Targeted Diversity Library

This library covers more than 1,000 targets and isoforms. 1-3 compounds with high potency and selectivity were carefully selected for each target and isoform. This library is a concise collection of small molecule compounds with comprehensive target coverage, which can be used for phenotypic screening at a low cost.

HY-L111 Novel Bioactive Compound Library

All compounds in this library have validated bioactivities tested by cell-based or biochemical assays. These compounds are structurally novel and bioactivity diverse, which makes it easier to discover new lead compounds.

Strength

- With a full range of product catalogs, including more than 20, 000 bioactive compounds.
- All compounds with high bioactivity and specificity are collected from literature and patents. The cell activity is general between nM to μM.
- Cover more than 1,000 kinds of targets. All compounds have explicit bioactive annotations.
- Most of the compounds have been tested in vivo and have good pharmacokinetic properties and stable metabolism.
- Specially designed to increase potential high-quality hits.
- With high structure diversities, including 136, 000+ Bemis-Murcko scaffolds. The average dissimilarity is 0.9.
- Re-supply of any hit-compound guaranteed from mg level to kg level.

Compound Screening Libraries

02. DRUG REPURPOSING RESEARCH

Drug repurposing is a new trend in drug development. Compared with new drug development, drug repurposing has the following advantages: Drug safety has been widely verified at the clinical stage and in the pharmaceutical market, which reduces the risk of drug development failure caused by safety.

Library Recommendation

HY-L022P **FDA-Approved Drug Library Plus**

A unique collection of compounds approved by the FDA, EMA, NMPA, and other countries. All compounds have completed extensive preclinical and clinical studies and have well-characterized bioactivities, safety, and bioavailability properties. It's a preferred library for drug repurposing.

Other Drug Repurposing Series

HY-L022
FDA-Approved Drug Library

HY-L066
FDA Approved & Pharmacopeial Drug Library

HY-L026
Clinical Compound Library

HY-L026P
Clinical Compound Library Plus

HY-L035
Drug Repurposing Compound Library

HY-L035P
Drug Repurposing Compound Library Plus

HY-L053
NMPA-Approved Drug Library

HY-L116
EMA-Approved Drug Library

HY-L112
Chemotherapy Drug Library

HY-L104
Children's Drug Library

HY-L140
Withdrawn Drug Compound Library

HY-L141
Off-Patent Drug Library

Publications Citing Use of MedChemExpress Compound Libraries

Nat Microbiol. 2023 Jan;8(1):121-134.
Cell Mol Immunol. 2023 Mar 2;1-14.
J Exp Med. 2023 Mar 6;220(3):e20221316.
Cell Rep. 2023 Feb 17;42(2):112105.
J Cell Biol. 2023 Jan 2;222(1):e202202110.
Int J Mol Sci. 2022 Apr 28;23(9):4891.
Cell Stem Cell. 2022 Apr 7;29(4):545-558.e13.
Nat Cancer. 2022 May;3(5):614-628.
JCI Insight. 2022 Aug 8;7(15):e160247.
Nat Commun. 2021 Jan 12;12(1):280.
Sci Adv. 2021 Dec 24;7(52):eabb3673.
Pharmacol Ther. 2021 Dec;228:107930.
Sci Adv. 2022 Oct 7;8(40):eabn9350.
EBioMedicine. 2022 Dec 8;87:104397.

Compound Screening Libraries

03.

DRUG DISCOVERY BASED ON NATURAL PRODUCTS

The structural diversity of natural products and their easy binding with biomacromolecules determine their incomparable advantages in the process of life regulation and endue natural products with an irreplaceable important position in the research and development of new drugs. Natural products and their molecular frameworks are the primary sources of new drugs.

Library Recommendation

HY-L021P Natural Product Library Plus

This library includes 4,500+ natural compounds containing Saccharides and Glycosides, Phenylpropanoids, Quinones, Flavonoids, Terpenoids and Glycosides, Steroids, Alkaloids, Phenols, Acids, and Aldehydes. Compounds in this library have high structural and 3-dimensionality (3D) diversity, with 2, 000+ Bemis-Murcko scaffolds and an average Fsp3 value of 0.51. All natural products have clear sources and structure classifications. This library is a comprehensive collection of natural products, a valuable tool for drug discovery based on natural products.

HY-L021L Natural Product-like Compound Library

This library includes nearly a thousand natural product-like compounds that are structurally like Steroids, Tannins, Flavonoids, Quinones, Isoquinolines, etc. This library is an important source of lead compounds for drug discovery.

Other Natural Products Series

HY-L021 Natural Product Library	HY-L115 Plant-Sourced Natural Product Library	HY-L065 Traditional Chinese Medicine Active Compound Library
HY-L056 Terpenoids Library	HY-L057 Phenols Library	HY-L068 Flavonoids Library
HY-L071 Alkaloids Library	HY-L055 Medicine Food Homology Compound Library	HY-L114 Anti-Inflammatory Traditional Chinese Medicine Active Compound Library
HY-L107 Anti-Cancer Natural Product Library	HY-L113 Antiviral Traditional Chinese Medicine Active Compound Library	HY-L143 Marine-Sourced Natural Product Library

Compound Screening Libraries

04.

DRUG DISCOVERY BASED ON STRUCTURE

Different product structures determine different functions. For example, compounds with covalent reactive groups can bind irreversibly to target through covalent bonds, which can lead to the development of highly selective inhibitors and overcoming drug resistance.

Library Recommendation

HY-L036P **Covalent Screening Library Plus**

This library contains 3, 000+ small molecules, including identified covalent inhibitors and other molecules having common covalent reactive groups as warheads, such as acrylamides, activated terminal acetylenes, sulfonyl fluorides/esters, cloracetamides, alkyl halides, epoxides, aziridines, disulfides, etc. This library is a valuable tool for covalent drug discovery.

Other Recommended Compound Libraries

HY-L036 Covalent Screening Library	HY-L138 Heterocyclic Compound Library	HY-L041 Macrocyclic Compound Library	HY-L033 Peptidomimetic Library
HY-L105 Peptide Library	HY-L110 Cyclic Peptide Library	HY-L042 Glycoside Compound Library	HY-L043 Lipid Compound Library
HY-L044 Nucleotide Compound Library			

Publications Citing Use of MedChemExpress Compound Libraries

Food Chem. 2023 Jul 1;413:135598.

Signal Transduct Target Ther. 2022 Aug 15;7(1):288.

Circulation. 2022 Apr 12;145(15):1154-1168.

Protein Cell. 2022 Sep 28;14(1):17-27.

Nat Commun. 2023 Mar 28;14(1):1726.

Nat Microbiol. 2023 Jan;8(1):121-134.

Free Radic Biol Med. 2023 Apr 10;203:86-101.

Circulation. 2022 Apr 12;145(15):1154-1168.

J Med Chem. 2022 Aug 25;65(16):11058-11065.

J Med Virol. 2021 Oct;93(10):5825-5832.

Cell Stem Cell. 2022 Apr 7;29(4):545-558.e13.

Cell Mol Immunol. 2023 Mar 2;1-14.

Compound Screening Libraries

05.

SCREENING BASE ON TARGETS AND SIGNALING PATHWAYS

Cell signaling pathways are involved in the pathophysiology of many diseases. The mutations, molecular damage, or functional change of the proteins in the signaling pathway will cause diseases. Therefore, knowledge of basic cell signaling mechanisms are essential to understand pathophysiologic and pharmacologic mechanisms.

MedChemExpress can supply more than 60, 000 bioactive compounds, covering 1, 000+ targets and 20+ hot signaling pathways, including GPCRs, Epigenetics, Immunology/Inflammations and cell proliferation, etc. These compounds are important tools for drug discovery based on targets and signaling pathways.

Cell Death Series

HY-L003 Apoptosis Compound Library	HY-L029 Autophagy Compound Library	HY-L051 Ferroptosis Compound Library
HY-L059 Pyroptosis Compound Library	HY-L133 Cuproptosis Compound Library	

Metabolism Series

HY-L012 Metabolism/Protease Compound Library	HY-L058 Glycolysis Compound Library	HY-L064 Glutamine Metabolism Compound Library
HY-L030 Human Endogenous Metabolite Compound Library	HY-L078 Gut Microbial Metabolite Library	HY-L084 Microbial Metabolite Library
HY-L123 Human Metabolite Library	HY-L091 Lipid Metabolism Compound Library	HY-L092 Glucose Metabolism Compound Library

According to Signaling Pathway or Protein Family

HY-L004 Cell Cycle/DNA Damage Compound Library	HY-L005 Epigenetics Compound Library	HY-L006 GPCR/G protein Compound Library

HY-L007 Immunology/Inflammation Compound Library	HY-L008 JAK/STAT Compound Library	HY-L009 Kinase Inhibitor Library
HY-L010 MAPK Compound Library	HY-L011 Membrane Transporter/ Ion Channel Compound Library	HY-L013 Neuronal Signaling Compound Library
HY-L014 NF-κB Signaling Compound Library	HY-L015 PI3K/Akt/mTOR Compound Library	HY-L016 Protein Tyrosine Kinase Compound Library
HY-L017 Stem Cell Signaling Compound Library	HY-L018 TGF-beta/Smad Compound Library	HY-L020 Wnt/Hedgehog/Notch Compound Library
HY-L024 Histone Modification Research Compound Library	HY-L037 Antioxidant Compound Library	HY-L038 Differentiation Inducing Compound Library
HY-L039 Reprogramming Compound Library	HY-L045 Oxygen Sensing Compound Library	HY-L050 Ubiquitination Compound Library
HY-L054 Endoplasmic Reticulum Stress Compound Library	HY-L060 Cytoskeleton Compound Library	HY-L062 Neurotransmitter Receptor Compound Library
HY-L072 Exosomes Compound Library	HY-L081 Phosphatase Inhibitor Library	HY-L088 Angiogenesis-Related Compound Library
HY-L089 Mitochondria-Targeted Compound Library	HY-L090 Transcription Factor-Targeted Library	HY-L095 Mechanoreceptors Compound Library
HY-L117 Calcium Channel Blocker Library	HY-L118 Sodium Channel Blocker Library	HY-L119 Potassium channel compound library
HY-L120 GABA Receptor Compound Library	HY-L121 5-HT Receptor Compound Library	HY-L126 Nuclear Receptor Compound Library
HY-L128 E3 Ligase Ligand Library	HY-L129 Target Protein Ligand Library	HY-L109 Protein-protein Interaction Inhibitor Library
HY-L131 Osteogenesis Compound Library	HY-L132 Chemokine Compound Library	HY-L136 Coagulation and Anticoagulation Compound Library

Compound Screening Libraries

06.

DRUG DISCOVERY BASED ON DISEASE

Based on the pathogenesis of different diseases, MedChemExpress carefully prepared some disease-related compound libraries, including Anti-Cancer Libraries, Anti-Infection Libraries, Neurodegenerative Disease Libraries and Other Disease Related Compound Libraries. These libraries consist of compounds with validated and potential bioactivity against respective diseases.

Anti-Cancer Series

HY-L025 Anti-Cancer Compound Library	HY-L031 Small Molecule Immuno-Oncology Compound Library	HY-L083 Anti-Cancer Metabolism Compound Library
HY-L080 Targeted Therapy Drug Library	HY-L112 Chemotherapy Drug Library	HY-L122 FDA-Approved Anticancer Drug Library
HY-L074 Anti-Breast Cancer Compound Library	HY-L075 Anti-Lung Cancer Compound Library	HY-L077 Anti-Pancreatic Cancer Compound Library
HY-L079 Anti-Blood Cancer Compound Library	HY-L101 Anti-Liver Cancer Compound Library	HY-L103 Anti-Colorectal Cancer Compound Library
HY-L124 Anti-Prostate Cancer Compound Library	HY-L135 Cancer Stem Cells Compound Library	HY-L107 Anti-Cancer Natural Product Library

Neurodegenerative Disease Series

HY-L085 Anti-Parkinson's Disease Compound Library	HY-L086 Neurodegenerative Disease-Related Compound Library	HY-L070 Neuroprotective Compound Library
HY-L069 Anti-Alzheimer's disease Compound Library		

Anti-Infection Series

HY-L002 Anti-Infection Compound Library	HY-L048 Antifungal Compound Library	HY-L049 Antibacterial Compound Library
HY-L067 Antibiotics Library	HY-L082 Antiparasitic Compound library	HY-L027 Antiviral Compound Library
HY-L052 Anti-COVID-19 Compound Library	HY-L073 Anti-Hepatitis C Virus Compound Library	HY-L113 Antiviral Traditional Chinese Medicine Active Compound Library
HY-L127 Anti-Orthopoxvirus Compound Library		

Other Disease Related Compound Libraries

HY-L125 Anti-Pulmonary Fibrosis Compound Library	HY-L130 Non-Steroidal Anti-Inflammatory Compound Library	HY-L034 Anti-Aging Compound Library
HY-L040 Diabetes Related Compound Library	HY-L046 Anti-Cardiovascular Disease Compound Library	HY-L047 Endocrinology Compound Library
HY-L087 Anti-Diabetic Compound Library	HY-L102 Rare Diseases Drug Library	HY-L108 Antidepressant Compound Library
HY-L134 Anti-Aging Natural Product Library	HY-L139 Pain-Related Compound Library	

Publications Citing Use of MedChemExpress Compound Libraries

Nat Commun. 2023 Mar 28;14(1):1726.
Plant Biotechnol J. 2023 Jan;21(1):63-77.
J Exp Clin Cancer Res. 2023 Feb 9;42(1):45.
Small. 2023 Apr;19(16):e2207194.
Cancer Immunol Res. 2023 May 3;11(5):583-599.
Food Chem. 2023 Jul 1;413:135598.
Sci Adv. 2023 Mar;9(9):eade3760.
J Transl Med. 2023 Mar 9;21(1):184.
Nat Cancer. 2022 May;3(5):614-628.

Compound Screening Libraries

07.

DRUG SCREENING BASED ON PRODUCT FEATURES

Different physico-chemical properties of the products determine their characteristics, and their applications in different research areas. For example, some compounds with low MW, fewer formal charges (particularly negative charges), and lower polar surface area tend to be more CNS-penetrant. CNS-penetrant compounds are important tools for the studying of neurological disorders, but they also have neurotoxicity.

Library Recommendation

HY-L028 CNS-Penetrant Compound Library

This library contains nearly 1,000 compounds with confirmed CNS-Penetrant properties. It's a valuable tool for the discovery of drugs used for brain diseases, such as brain tumors, mental disorders, and neurodegenerative diseases.

HY-L061 Orally Active Compound Library

Most drugs available in the marketplace are administered via the oral route, which is a convenient and cost-effective route of administration. Thus, oral bioavailability is one of the critical considerations in drug design and development. **MedChemExpress** offers a unique collection of 3,000+ compounds with confirmed high oral bioavailability. **MedChemExpress** Orally Active Compound Library is a valuable tool for discovering new drugs with oral bioavailability.

Other recommended Compound Libraries

HY-L023 Toxins for Antibody-Drug Conjugate Research Library	HY-L100 Tumorigenesis-Related Compound Library	HY-L094 Food-Sourced Compound Library
HY-L063 Chemical Probe Library	HY-L076 Drug-Induced Liver Injury(DILI) Compound Library	HY-L093 Food Additive Library
HY-L096 Inactive Ingredient Library	HY-L097 Animal Disease Model Inducer Library	HY-L098 Drug Metabolite Library
HY-L137 Molecular Glue Compound Library	HY-L151 PROTAC Library	

Compound Screening Libraries

08. DIVERSITY COMPOUND LIBRARIES

It is proved that a diverse compound library is the most successful and straightforward starting point to discover new leads because it contains highly dissimilar new chemical scaffolds. **MedChemExpress** can provide a series of diverse compound libraries.

Library Recommendation

HY-L901 50K Diversity Library

A representative diversity set, average Tanimoto coefficient of 0.508. Highly recommended for random screening against new as well as popular targets based on its novel, diverse scaffolds, abundant chemical spaces and the convenience for subsequent modification.

HY-L902 5K Scaffold Library

An exceptionally diverse library, each compound represents one unique scaffold. The sufficient diversity of compound structure makes this library a powerful tool for preliminary hits screening.

HY-L903 3D Diverse Fragment Library

This library comprises 5,196 non-flat fragment-like compounds and is designed based on 3D structure for structural diversity and reactivity. This brings higher fragment hit optimization and increases the likelihood of finding innovative hits in FBDD.

HY-L910V 50K Virtual Diversity Library

A novel collection of 50,000 synthetically accessible, lead-like compounds with exceptional structural diversity. Compounds in this library are easy to synthesize via standard 1-2 step procedures.

HY-L912V 10M Virtual Diversity Library

A unique collection contains 10,000,000 synthetically accessible screening compounds. This library is highly recommended for AI-based lead discovery, ultra-large virtual screening, and novel lead discovery.

High throughout libraries with more than 26 million compounds

These libraries come from different internationally renowned brands. They are not only suitable for virtual screening, but also for various in vitro drug screening experiments for new drug discovery.

Compound Screening Libraries

09. DEL LIBRARY

DNA Encoded Compound Library (DEL) technology has emerged as an enabling tool in the drug discovery field; featured an incredibly convenient and rapid way to assess the binding affinity of billions of chemical compounds and discover potential ligands for biological and pharmaceutical interested protein targets. Based on more than 50,000 high-quality building blocks, combined with hundreds of DNA-compatible reactions, **MedChemExpress** synthesized a series of DNA-encoded libraries consisting of billions of compounds with abundant chemical spaces and novel structures.

3 Kits

DEL A Kit

20 DEL libraries, covering over 300 million DEL molecules, 1 tube set

DEL B Kit

50 DEL libraries, covering over 1 billion DEL molecules, 1 tube set

DEL T Kit

68 DEL libraries, covering over 2 billion DEL molecules, 1 tube set

Mini DEL library

DEL C Kit Covalent library

5 DEL libraries, covering over 3 million DEL molecules, 1 tube set

DEL D Kit Cyclic peptide library

5 DEL libraries, covering over 8 million DEL molecules, 1 tube set

DEL E Kit Regular library

5 DEL libraries, covering over 190 million DEL molecules, 1 tube set

DEL F Kit Regular library

5 DEL libraries, covering over 109 million DEL molecules, 1 tube set

DEL G Kit Regular library

5 DEL libraries, covering over 113 million DEL molecules, 1 tube set

DEL H Kit Regular library

10 DEL libraries, covering over 550 million DEL molecules, 1 tube set

DEL Library Customized Service

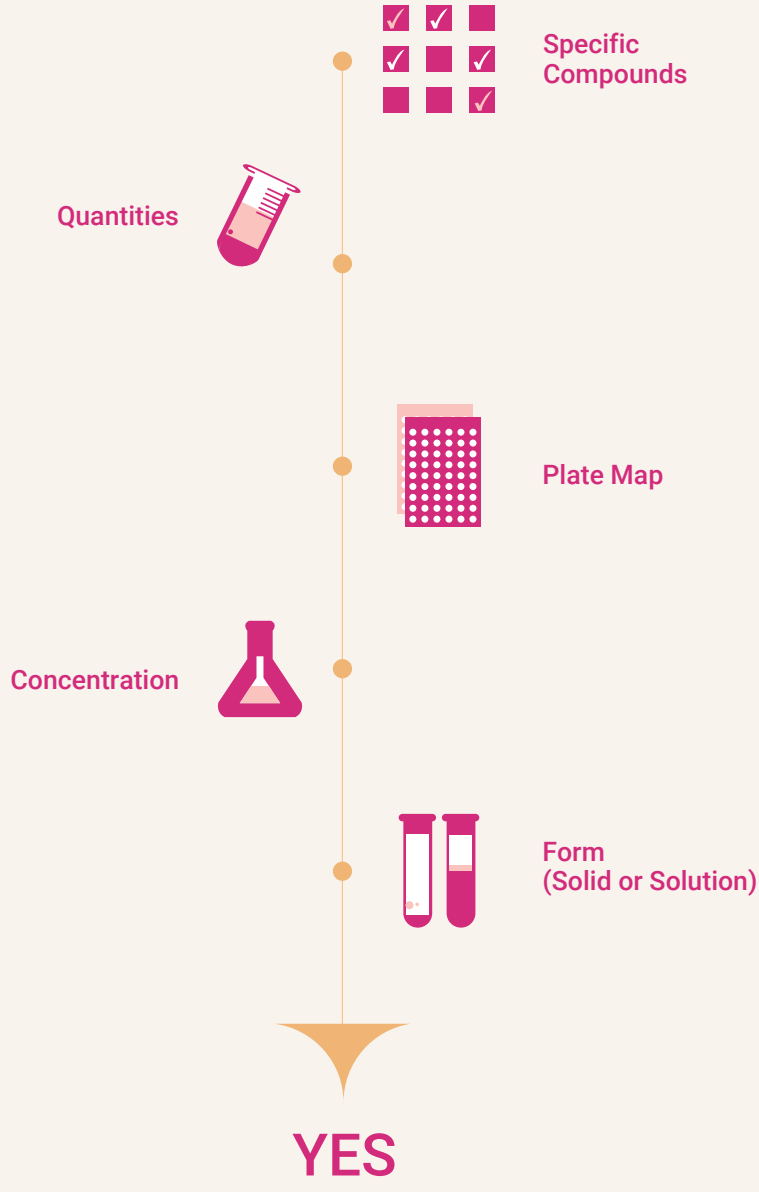
Depending on the specific building block structure of your request, **MedChemExpress** can provide customized DEL synthesis service. Through the use of cutting-edge technologies, **MedChemExpress**'s robust and professional DEL synthesis team have been developed more than 100 different types of chemical reactions in the presence of a DNA tag.

Compound Screening Libraries

10.

CUSTOMIZE YOUR LIBRARIES

Any customization can be made according to your needs



Compound Screening Libraries

11
CASE STUDIES

MedChemExpress Anti-cancer Compound Library Assisted the Mechanism Study and Drug Discovery of Sox10-deficient Melanomas

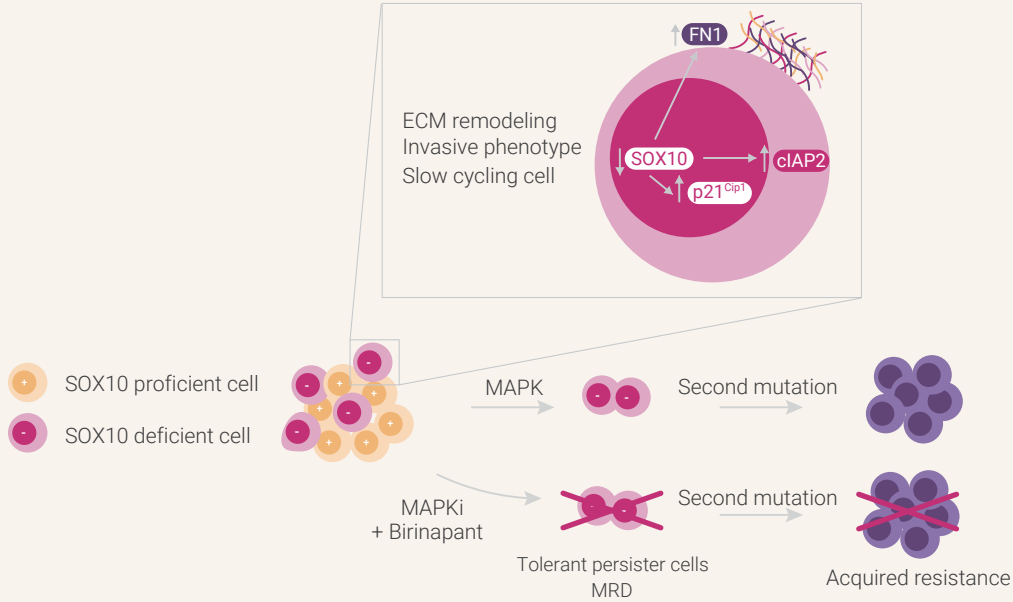
Background

SOX10 is heterogeneously expressed in melanomas. Loss of SOX10 reduces proliferation, leads to invasive properties, and promotes tolerance to BRAF and/or MEK inhibitors. After taking high throughput screening using **MedChemExpress** anti-cancer library (Cat. No: HY-L025), all five cIAP1/2-XIAP inhibitors included in the screen effectively induced cell death in SOX10 knockout cells with little-to-no effect on parental cells. Thus, cIAP1 and/or cIAP2 may be relevant targets for causing cell death in SOX10 knockout cells.

Further studies showed that cIAP2 is a crucial target for inducing cell death in SOX10 knockout cells.

Conclusion

cIAP1/2 inhibitors can delay the onset of acquired resistance to BRAF/MEK inhibitors in melanomas *in vivo*.



Nat Commun. 2022 Mar 16;13(1):1381.

MedChemExpress Compound Library Assists in Building of NIH Screening Platform

The NIH Chemical Genomics Center (NCGC) is an ultrahigh-throughput screening center of the Molecular Libraries Probe Production Centers Network (MLPCN) that owns advanced HTS equipment and testing instruments. **MedChemExpress** continuously supplies tens of thousands of compounds to the platform, some of which are hundreds of milligrams in size, providing strong support for its platform building and maintenance.

NIH National Institutes of Health

MedChemExpress Compound Library Powers the Disease Study of St. Jude Children's Research Hospital

St. Jude Children's Research Hospital (St. Jude) is a comprehensive research center designated by the National Cancer Institute for the treatment of childhood cancer, with rich experience in basic research and clinical transformation in pediatric disease research.

In recent years, **MedChemExpress** has established a stable cooperation relationship with St.Jude as a quality supplier to the Screening Center of St. Jude; continuously supplies dozens of compound libraries, with tens of thousands of compounds, it supports drug discovery and disease research at St. Jude.

St. Jude Children's® Research Hospital
Finding cures. Saving children.

MedChemExpress Compound Libraries Promote Drug Discovery in the Early Stage

MedChemExpress compound Libraries have been widely recognized by large pharmaceutical companies worldwide. **MedChemExpress** has become a stable supplier of pharmaceutical enterprises and continuously supplies a large number of high-quality compound libraries for accelerating drug early development.

Roche Lilly MSD Johnson & Johnson
GSK AMGEN GILEAD Genentech
AstraZeneca abbvie Incyte LEO

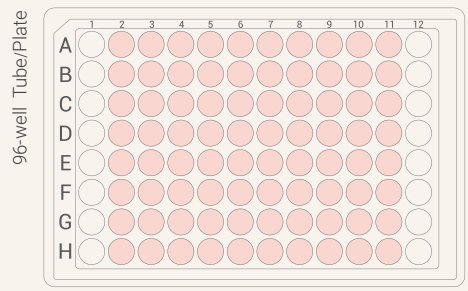
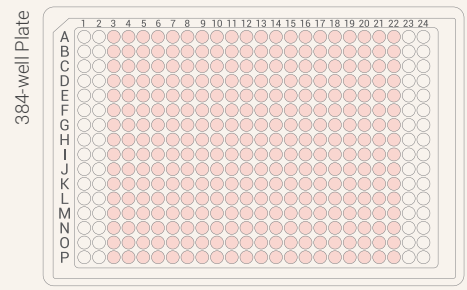
Compound Screening Libraries

12.

PARAMETERS OF MCE BIOACTIVE COMPOUND LIBRARY

96-well Format Sample Storage Tube

96-/384- well Plate

Specifications	30 μL, 50 μL, 100 μL or other size lower than 500 μL	30 μL, 50 μL, 100 μL or other size lower than 100 μL
Sealing Way	Screw Cap	Peelable Foil Seal
Concentration	**10 mM** solution for products with stable solution state and solubility no less than 10 mM; **2 mM** solution for products with solubility between 2 mM and 10 mM; **3 mg/mL** solution for products with unconfirmed molecular weight and solubility no less than 3 mg/mL	
Solvent	DMSO, Water, Ethanol	
Recommended Storage Time	Powder: -20°C (3 years); 4°C (2 years) In solvent: -80°C (2 years); -20°C (1 year)	
Information Shipped with Library	**Product information** including targets, bioactivity information, research areas, clinical data, etc.; **Product layout** for each plate; **SDF file**, contains structure information and requires some specialized software to open (ChemOffice).	
Plate Layout	 Compounds  Empty Compounds with different concentrations or dissolved in different solutions are put on separate plates. If you have any other requirements for the layout of compounds, please let us know before you make the order.	

VIRTUAL SCREENING

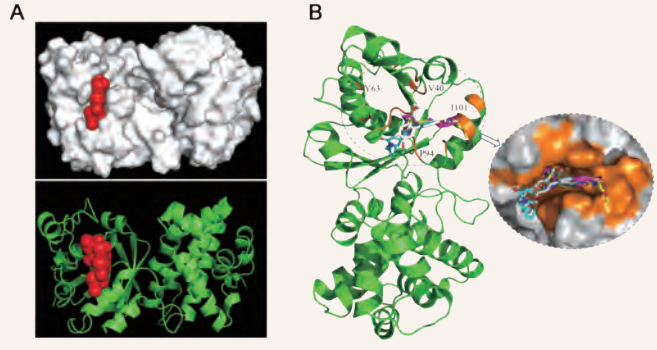
Virtual Screening is an effective tool for rapidly screening of millions of compounds with reasonable binding patterns and potential druggability. It is based on the molecular docking of compounds in the druggable pocket on a target protein. It can bypass primary wet-lab screening hence, reducing the time and cost of novel drug discovery.

Advantages

- High-performance computer servers
- All kinds of different libraries (>16 million compounds)
- High standard intellectual property management (confidentiality)
- Experienced professionals for molecular docking and drug design
- SCI publishable 2D/3D molecular docking figures can be provided

Example

Virtual screening for the discovery of GPD1 allosteric activator and analysis of the GPD1-compound binding model.



A. Crystal structure of GPD1 protein (PDB ID:6E8Y).
Red represents the predicted allosteric sites.
B. Representation of GPD1 protein with compounds discovered by virtual screening.

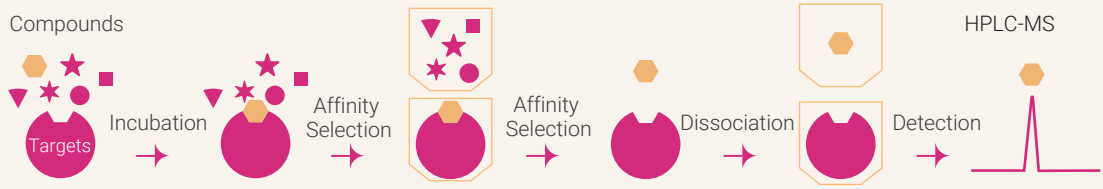
J Hematol Oncol. 2022 Jul 14;15(1):93.

DRUG SCREENING SERVICES

01.

AS-MS SCREENING

MedChemExpress offers AS-MS (Affinity Selection-Mass Spectrometry) screening to support the identification of compounds with strong affinity and specificity for a target protein, which could be a perfect starting point for your novel drug discovery projects.



AS-MS Screening Process

Advantages

- Several successful projects with repeatability and high consistency
- Customized and cost-effective service
- High standard intellectual property management (confidentiality)
- Experienced professionals and cutting-edge facility

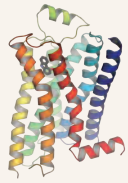
02.

TARGET BASED SCREENING (GPCR/ KINASE/ ION CHANNEL)

Around half of the approved drug targets are GPCRs, kinases, ion channels, and nuclear receptors, and 70% of the approved small molecule drugs are targeted against these four types. **MedChemExpress** can do compound screening with hundreds of stable cell lines specifically for GPCRs and ion channels. For kinase screening & profiling, we can provide both in vitro and in vivo screening services. A bunch of different screening methods would be customized based on your requests.

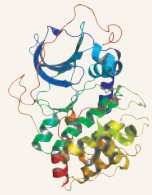
30+ Ion Channel Assay Models

- Platforms of different throughputs: Qpatch16X, QpatchHTX, IonWorks Barracuda
- Gold standard: manual patch clamp
- Fluorescent platform: FLIPR, FDSS/μCell



100+ GPCR Stable Cell Lines

- Multiple assays formats, including calcium flux, cAMP determination
- FLIPRPENTA (EMC-CD), BMGPHERAstar FSX, BIOTEK multifunctional plate reader
- Customized GPCR stable cell line construction



400+ Kinase

- A long list of kinas: AGC, CAMK, CMGC, CK1, STE, and common mutants
- Flexible and customizable kinase panel: 60/207/302 kinase panels and customized kinase panels
- Various detection: TR-FRET, fluorescence, Z`-LYTE, binding assay

03.

ANTI-CANCER COMPOUND SCREENING IN VITRO

MedChemExpress compound activity screening (anti-cancer compound screening in vitro) platform takes the whole cell as the research object, and can provide a variety of cell proliferation and cytotoxicity detection services. We can also detect the effect of compounds on cell apoptosis, cell cycle to obtain a large amount of relevant information from a single experiment, determine the biological activity and potential toxicity of the compound.

Advantages

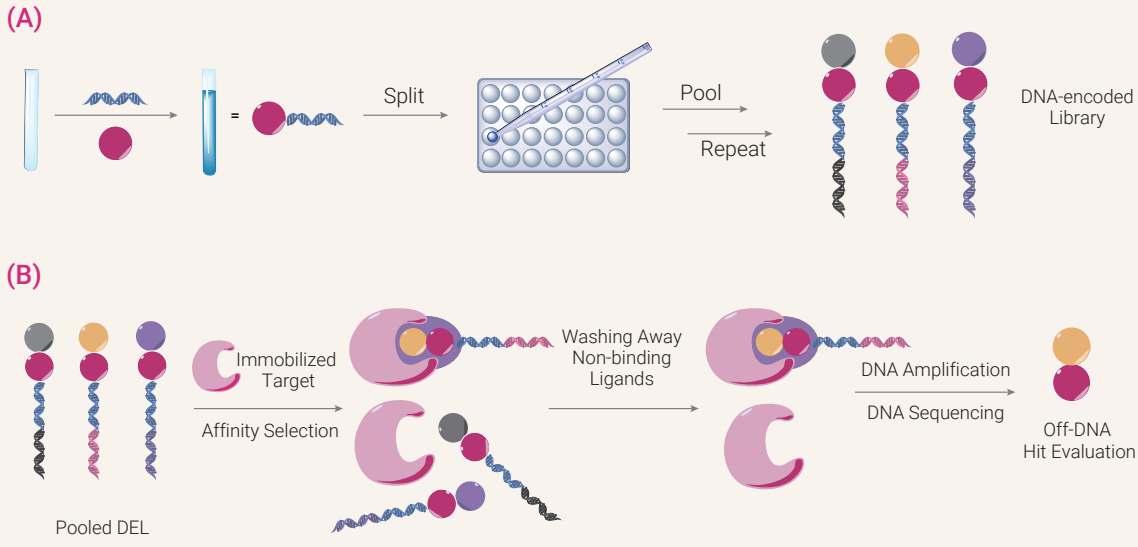
- 120+ tumor cell lines
- A variety of cell viability assays
- The professional compound screening team
- Experienced professionals and high resolution imaging system
- Advanced equipments

04.

DEL SCREENING

MedChemExpress's one-stop DEL screening platform consists of not only a series of in-stock DEL libraries such as photo-cross-linking DELs, covalent DELs, cyclic peptide DELs, but also DEL customized service, and DEL screening service.

Customized DEL synthesis service can be provided depending on any specific building block structure request. Through the use of cutting-edge technologies, **MedChemExpress**'s strong and professional DEL synthesis team has developed more than 100 different types of chemical reactions in the presence of DNA tag.



Overview of DNA-Encoded Library (DEL) Technology.
(A) DEL Synthesis. (B) DEL Screening.

Advantages

- 68 DEL libraries, covering billions of DEL molecules.
- Novel chemical structure, comprehensive chemical space coverage, and drug-like molecular characteristics
- Strict quality control and verification system
- Tailor-made DEL library
- Keep up with research trends and keep updating
- A small amount of protein sample: about 100 μg protein (depending on the protein's molecular weight)
- Short lead time and high cost performance

LEAD COMPOUND OPTIMIZATION

Lead compounds obtained by high-throughput screening may have problems, such as high toxicity, poor metabolic stability in vivo, and low bioavailability. So the structures need to be further optimized. **MedChemExpress** can provide lead compound analogs search and supply, custom synthesis, chemical analysis, and detection services.

01. SEARCH AND SUPPLY OF STRUCTURE ANALOGS

- Deep analysis of screening hits and hit classification into chemical families
- Search for structural analogs in the available chemical space
- Supply and custom synthesis of structural analogs

02. CUSTOM SYNTHESIS

MedChemExpress is committed to the custom synthesis of complex compounds with high challenges. **MedChemExpress** has built an experienced chemical synthesis team with hundreds of advanced equipment, and established a set of perfect custom synthesis service systems, which can scale up from milligrams to kg scale to meet different customer needs.

03. ANALYTICAL DEVELOPMENT & QUALITY CONTROL

- R&D testing
- Analytical method development and validation
- Impurity preparation, separation, and purification
- Genotoxic impurity research
- Structure characterization and impurity analysis
- Stability study
- Registration application services

Inhibitors • Screening Libraries • Proteins

www.MedChemExpress.com

Service and Distribution in Germany

BIOZOL
FIT FOR SCIENCE

www.biozol.de | info@biozol.de

MedChemExpress USA

Tel: 609-228-6898 **E-mail:** sales@MedChemExpress.com
Fax: 609-228-5909 **Tech Support:** tech@MedChemExpress.com
Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA

MedChemExpress Europe

Tel: + 46 86500910 **E-mail:** eu.sales@MedChemExpress.com
Address: Bergkällavägen 37C, 192 79 Sollentuna, SWEDEN