

CAS BIOFINDER DISCOVERY PLATFORM™

快速使用指南 (QUICK GUIDE)



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提纲

- CAS BioFinder 简介与检索界面介绍 (Introduction and Interface)
- 配体检索与配体详情信息 (Ligands and Details Overview)
- 骨架检索与构效关系分析 (Scaffolds and SAR Analysis)
- 蛋白/通路/靶点、疾病与生物标志物 (Proteins & Pathways; Diseases & Biomarkers)
- 生物活性预测 (Predictive Analytics)

科学信息管理对新药研发至关重要

低增长时代的特点对创新的要求极大提升，而在当今的创新环境下，数据管理任务艰巨

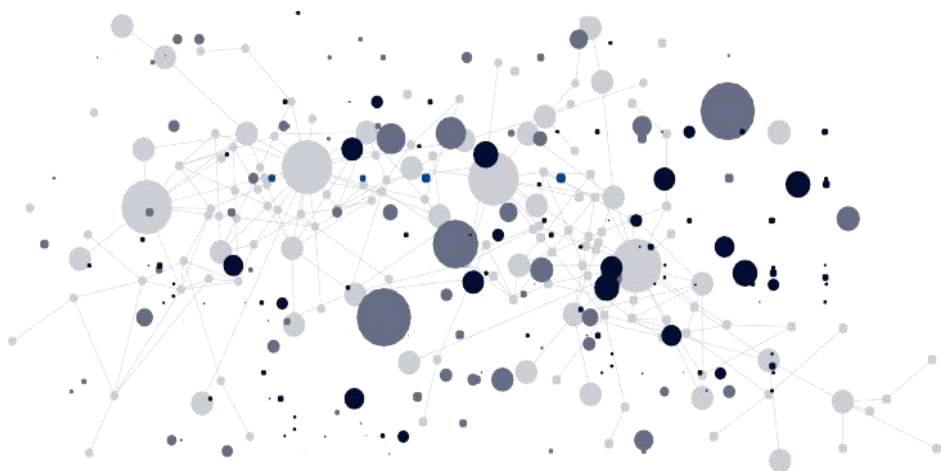
- 信息鸿沟会导致创新管线薄弱、研发效率低下，以及意外的知识产权风险
- 由于数据量和数据类型日益复杂，药物发现流程中，整合和分析关键的研发数据信息，对于迅速做出关键决策至关重要。
- 持续的数据管理有助于开发差异化的成果，支撑创新药物的发现，确保药物研发成功进入审批阶段，并可避免后续知识产权问题。

来源：CAS Insights洞察报告 [Challenges and opportunities in data for drug discovery | CAS](#)

生命科学领域研究离不开重要的数据信息基础， 但为什么却难以加以利用？

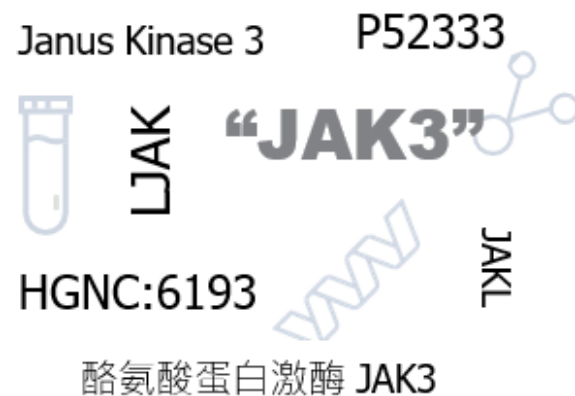
缺乏关联性

生命科学研究和数据分散在各个数据库、
期刊和专利等众多互不关联的资源之中



未一致化

不同资源对相同信息的描述各不相同，
因此很难对数据进行分析 and 比较



数据问题导致延缓创新进程， 增加财务风险

遗漏见解



这些见解能够为研究人员制定研发战略提供指导

仅在美国， 每年就有 **5,000 到 6,000 起专利侵权和专利无效**的诉讼， 法院判定的**赔偿金额接近 50 亿美元**¹。

耗费时间



生命科学数据量每 **14 年翻一番**²

数据科学家将 **50%-80% 的时间都花费**在收集和整理用于分析模型的数据信息的琐碎的工作中³

1. Vuleta, B. (2023). 25 Patent Litigation Statistics - High-Profile Feuds about Intellectual Property. LegalJobs. <https://legaljobs.io/blog/patent-litigation-statistics/>

2. Bornmann, L. et al. (2021). Growth rates of modern science: a latent piecewise growth curve approach to model publication numbers from established and new literature databases. (Humanities and Social Sciences Communications), 8, 224. <https://doi.org/10.1057/s41599-021-00903-w>

3. Lohr, S. (2014.) For Big-Data Scientists, 'Janitor Work' Is Key Hurdle to Insights. The New York Times. August 17, 2014. <https://www.nytimes.com/2014/08/18/technology/for-big-data-scientists-hurdle-to-insights-is-janitor-work.html>

4. Genetic Engineering & Biotechnology News Top 25 Biotech Companies of 2019. 5. Pharm Exec's Top 50 Companies 2020.6. Shanghai Ranking's Global Ranking of Academic Subjects 2020.

利用CAS BioFinder 加速早期药物研发



CAS BioFinder 检索界面

The screenshot shows the CAS BioFinder web interface. At the top, the logo and navigation icons are visible. The main header area includes a greeting 'Good Afternoon,' and a search bar with a 'Draw' button. Below the search bar, there are tabs for 'Ligands', 'Scaffolds', 'Proteins', and 'Diseases'. A 'Predictive Analytics' section is also present. The bottom section shows the 'Recent Search History' with a table of search results.

Good Afternoon,

配体、骨架、蛋白/靶点、疾病检索（基于药物名称、CAS RN、结构、靶点、疾病）

Ligands Scaffolds Proteins Diseases

Search by protein, ligand, disease or draw a structure.

Draw

结构绘制面板

Predictive Analytics
Upload and analyze ligand data sets using algorithms to find bioactivity data insights.

活性预测分析（基于算法，预测某一个或多个结构与不同靶点的生物活性数据）

Recent Search History 近期检索历史

View Search History

3 September 2025

Proteins	KDR
3:51 PM	8 Results

Rerun Search

Edit search
Delete search

提纲

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- 生物活性预测 (Predictive Analytics)

基于靶点、疾病、药物名称以及结构，检索配体信息

Ligands Scaffolds

BTK
IBTK
Tyrosine-protein kinase BTK
Tyrosine-protein kinase BTK/M
BTKh
BTK Orange II
BTK Black 10BX
BTK Victoria Blue
BTK deficiency

自动提示叙词表

Filters

Chemical Filters

☐ Rule of 5 Filter Preset
This will automatically be applied.

☒ pValue

☒ Modality

☒ Druglikeness

☒ ADME

☒ Commercial Availability

☒ Approval Status

☒ Approval Authority

Biological Filters

☒ Target

☒ Target Type

☒ Disease

Ligands search for BTK

Ligands Scaffolds Pharmacology

29,502 Results

Sort: Relevance

Relevance

CAS RN: Ascending
CAS RN: Descending
Number of Targets: Ascending
Number of Targets: Descending
Number of Metabolites: Ascending
Number of Metabolites: Descending
Suppliers

检索结果排序

药物情报信息标识

1 936563-96-1 Ibrutinib
Metabolites: 3 | Proteins: 687

2 1420477-60-6 4-[8-Amino-3-[(2S)-1-(1-oxo-2-butyn-1-yl)-2-pyrrolidinyl]imidazo[1,5-σ]pyrazin-1-yl]-2-(4-phenoxyphenyl)-N-methyl-N-(2-oxo-2-propen-1-yl)pyrazol-1-amine
Metabolites: 0 | Proteins: 203

3 1691249-45-2 (7S)-4,5,6,7-Tetrahydro-7-[1-(1-oxo-2-propen-1-yl)-4-piperidinyl]-2-(4-phenoxyphenyl)-N-methyl-N-(2-oxo-2-propen-1-yl)pyrazol-1-amine
Metabolites: 0 | Proteins: 36

4 910232-84-7 N-[3-[4,5-Dihydro-4-methyl-6-[[4-(4-oxo-2-propen-1-yl)-1H-pyrazol-1-yl]-2-phenyl]-1H-pyrazol-1-yl]-4-methyl-1H-pyrazol-1-yl]-N-methyl-N-(2-oxo-2-propen-1-yl)pyrazol-1-amine
Metabolites: 7 | Proteins: 215

5 2095280-64-9 N-[3-[1,6-Dihydro-1-methyl-5-[[4-(4-oxo-2-propen-1-yl)-1H-pyrazol-1-yl]-2-phenyl]-1H-pyrazol-1-yl]-4-methyl-1H-pyrazol-1-yl]-N-methyl-N-(2-oxo-2-propen-1-yl)pyrazol-1-amine
Metabolites: 0 | Proteins: 203

6 2095280-65-0 N-[3-[1,6-Dihydro-1-methyl-5-[[4-(4-oxo-2-propen-1-yl)-1H-pyrazol-1-yl]-2-phenyl]-1H-pyrazol-1-yl]-4-methyl-1H-pyrazol-1-yl]-N-methyl-N-(2-oxo-2-propen-1-yl)pyrazol-1-amine
Metabolites: 0 | Proteins: 203

7 1803358-13-5 N-[2-Methyl-5-[2-oxo-9-(1H-pyrazol-1-yl)-1H-pyrazol-1-yl]-1H-pyrazol-1-yl]-N-methyl-N-(2-oxo-2-propen-1-yl)pyrazol-1-amine
Metabolites: 0 | Proteins: 36

8 910232-84-7 N-[3-[4,5-Dihydro-4-methyl-6-[[4-(4-oxo-2-propen-1-yl)-1H-pyrazol-1-yl]-2-phenyl]-1H-pyrazol-1-yl]-4-methyl-1H-pyrazol-1-yl]-N-methyl-N-(2-oxo-2-propen-1-yl)pyrazol-1-amine
Metabolites: 7 | Proteins: 215

筛选具有类似先导化合物特性的小分子配体

一键应用Rule of 5

Chemical Filters

☒ Rule of 5 Filter Preset
This will automatically be applied.

ADME

Partition Coefficient (logP)
-1.17 to 7.18
-1.17 to 5.00

Solubility (logS)
-8.94 to 0.58
-8.94 to 0.58

Blood-Brain Barrier Permeability (logBB)
-1.94 to 0.99
-1.94 to 0.99

Permeability Glycoprotein (Pgp)
0 to 1
0 to 1

Polar Surface Area (PSA) (Å²)
20 to 208
20 to 140

Plasma Protein Binding (PPB)
16 to 100
16 to 100

Modality

Druglikeness

Hydrogen Bond Acceptors
2 to 13
2 to 10

Hydrogen Bond Donors
0 to 7
0 to 5

Freely Rotatable Bonds
0 to 13
0 to 10

Molecular Weight (g/mol)
260 to 587
260 to 500

Molar Refractivity (m³/mol)
58 to 152
58 to 130

Number of Atoms
11 to 36
20 to 36

[Reset Filter](#) [Apply](#)

Ligands search for BTK

Ligands Scaffolds Pharmacology

Applied Filters (8) Hydrogen Bond Acceptors: 0 to 10 X Hydrogen Bond Donors: 0 to 5 X Freely Rotatable Bonds: 0 to 10 X Molecular Weight (g/mol): 0 to 500 X Molar Refractivity (m³/mol): 40 to 130 X

Partition Coefficient (logP): up to 5 X Polar Surface Area (PSA) (Å²): 0 to 140 X

9,273 Results

1 [936563-96-1](#)
Ibrutinib

Metabolites: 3 | Proteins: 687

2 [1202757-89-8](#)
CC 292

Metabolites: 7 | Proteins: 215

3 [1803358-13-5](#)
N-[2-Methyl-5-[2-oxo-9-(1H-pyrazol-1-yl)benzo[h]-1,6-naphthyridin-1(2H)-yl]phenyl]...

Metabolites: 7 | Proteins: 16

5 [1803358-31-7](#)
N-[2-Methyl-5-[2-oxo-9-(1H-pyrazol-1-yl)benzo[h]-1,6-naphthyridin-1(2H)-yl]phenyl]...

Metabolites: 8 | Proteins: 15

6 [1202755-92-7](#)
N-[3-[[5-Methyl-2-(phenylamino)-4-pyrimidinyl]amino]phenyl]-2-propenamide

Metabolites: 12 | Proteins: 12

7 [302962-49-8](#)
Dasatinib

Metabolites: 4 | Proteins: 733

9 [1415823-49-2](#)
1-[4-[[[6-Amino-5-(4-phenoxyphenyl)-4-pyrimidinyl]amino]methyl]-...

Metabolites: 12 | Proteins: 12

10 [1202755-89-2](#)
(2E)-4-(Dimethylamino)-N-[3-[5-fluoro-4-[(3-methylphenyl)amino]-...

Metabolites: 12 | Proteins: 12

11 [1202757-97-8](#)
1-[[[3R]-3-[[5-Fluoro-2-[(3-methoxyphenyl)amino]-4-pyrimidinyl]oxy]-...

Metabolites: 4 | Proteins: 733

- 氢键受体 <10
- 氢键供体 <5
- 自由旋转键 <10
- 分子量 <500
- 摩尔折射率：
40-130 m³/mol
- 原子数: 20-70
- logP <5
- 极性表面积：
0-140 Å²

配体检索结果的纵览与聚焦

可通过检索进行筛选聚焦

靶点

疾病

有机体

参数功能

实验类型

小分子

蛋白/肽类

配合物

抗体

ADC

聚合物

Approval Status

Modality

Ligands search for BTK

Filters

Chemical Filters

Biological Filters

Source Filters

Applied Filters (1) Target: Tyrosine-protein kinase BTK

Results

936563-96-1 Ibrutinib

2095280-64-9 N-[3-[1,6-Dihydro-1-methyl-5-[[4-(4-morpholinylcarbonyl)-3-[(1-oxo-2-propen-1-yl)...

2095280-65-0 N-[3-[1,6-Dihydro-1-methyl-5-[[4-(4-morpholinylcarbonyl)-3-[(1-oxo-2-propen-1-yl)...

2101700-15-4 5-Amino-3-[4-[[[5-fluoro-2-methoxybenzoyl]amino]methyl]phenyl]-1-[(1S)-2,2,2-tri...

1803358-31-7 N-[2-Methyl-5-[2-oxo-9-(1H-pyrazol-1-yl)benzo[h]-1,6-naphthyridin-1(2H)-yl]phenyl]...

1202755-92-7 N-[3-[[5-Methyl-2-(phenylamino)-4-pyrimidinyl]amino]phenyl]-2-propenamide

纵览配体检索结果集相关骨架结构与药理学数据

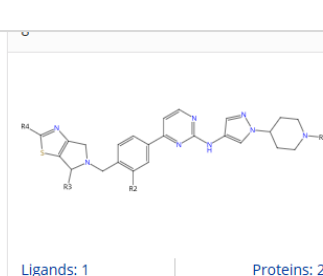
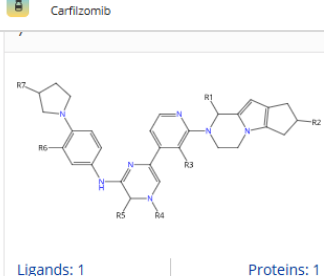
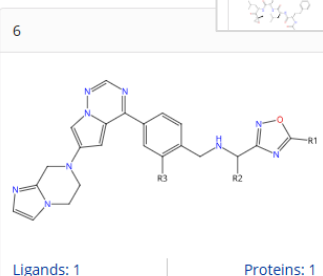
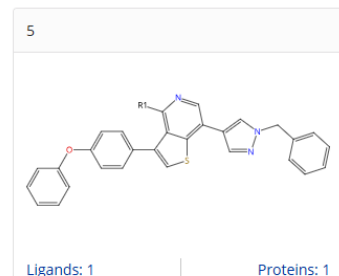
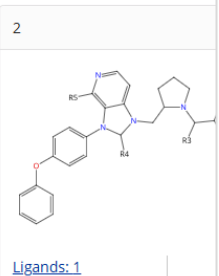
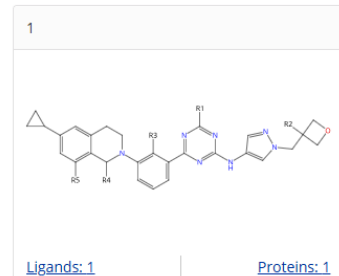
查看配体检索结果
关联的骨架结构

Ligands search for BTK

Ligands **Scaffolds** Pharmacology

Applied Filters (1) Target: Tyrosine-protein kinase BTK X Clear all filters

10,870 Results

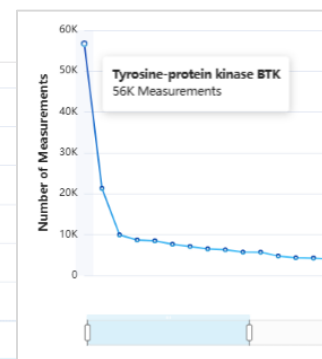
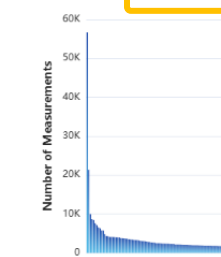


数据可视化:

- 柱状/折线图: 每条柱形/折线节点代表针对不同靶点的测量实验数量
- 调节图下方的横条, 可放大图表的特定区域

Ligands search for BTK

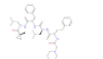
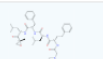
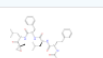
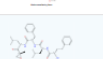
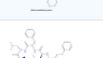
Ligands Scaffolds **Pharmacology**



Show Structures

ON

显示配体结构

	Target	Gene	Parameter	pValue	Value	Function	Assay	Source
	MV4-11 cell (Cell line)	-	IC50	17.06	8.67×10^{-12} μ M	Inhibitor	View	ChemMedChem (2019), 14(23), 2005-2022
	MV4-11 cell (Cell line)	-	IC50	16.88	1.33×10^{-11} μ M	Inhibitor	View	ChemMedChem (2019), 14(23), 2005-2022
	MV4-11 cell (Cell line)	-	IC50	16.63	2.34×10^{-11} μ M	Inhibitor	View	ChemMedChem (2019), 14(23), 2005-2022
	MV4-11 cell (Cell line)	-	IC50	16.50	3.15×10^{-11} μ M	Inhibitor	View	ChemMedChem (2019), 14(23), 2005-2022
	THP-1 cell (Cell line)	-	IC50	16.40	4.01×10^{-11} μ M	Inhibitor	View	ChemMedChem (2019), 14(23), 2005-2022

可下载表格中的
详细数据

点击View, 可查看原文
中的Assay的细节

探索配体的详细信息

Doxorubicin

CAS Registry Number: 23214-92-8

112K

1,642

Retrosynthesis

Predictive Analytics

...

View Associated Scaffold

View in CAS SciFinder

链接到CAS SciFinder
查看关联信息

SummaryPharmacologyADMEToxicologyProteins (313)Diseases (301)Related Immunotherapeutics (12)Chemical SpaceMetabolites (4)Similar Ligands (764)

配体相关信息标签页

药物情报信息

CAS DRUG INTELLIGENCE

Approved Drug

Doxorubicin is an antineoplastic in the anthracycline class. General properties of drugs in this class include: interaction with DNA in a variety of different ways including intercalation (squeezing between the base pairs), DNA strand breakage and inhibition with the enzyme topoisomerase II. Most of...

View More

STATUS

Approval Status: US Approved
Approval Authority: US FDA
Approval Year: 1974, 2024
Originator: Farmitalia

INDICATIONS

Ovarian cancer
Modality: Primary
Highest Phase: Approved
Source

PRIMARY TARGET

DNA topoisomerase II
Function: Inhibitor
Measurement: IC50 2.67 μM
Source

View AllView Related Drugs

配体属性信息

H bond acceptors*
12

H bond donors*
7

Molecular weight (g/mol)
543.52

Molar refractivity (m³/mol)
133.94

Number of atoms
39

Freely rotatable bonds*
5

logP*
0.918

logS
-3.27

logBB
-1.96

Polar surface area (Å²)*
206.07

Plasma protein binding
67.32

Permeability glycoprotein
1

* Calculated using Advanced Chemistry Development (ACD/Labs) Software (© 1994-2025 ACD/Labs)

Canonical SMILES

22 other names for this Ligand

配体结构信息与其他名称

药物情报信息 (Drug Intelligence)

CAS DRUG INTELLIGENCE

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View All

PRIMARY TARGET

DNA topoisomerase II

Function: Inhibitor
Measurement: IC50 2.67 µM
Source

View All

Targets

View Related Drugs

相关靶标

Primary Target	Function	Measurement
DNA topoisomerase II	Inhibitor	IC50 2.67 µM
Albumin	Binding Agent	-
DNA gyrase	Inhibitor	-
DNA topoisomerase II	Inhibitor	IC50 2.67 µM
A673	Inhibitor	IC50 200.0 nM
HepG2	Inhibitor	IC50 24.68 µM
Human ovarian cancer cell line	Inhibitor	IC50 0.074 µM

Indications

相关适应症

所处临床阶段和获批信息

×

Name	Modality	Highest Phase	Source
Ovarian cancer	Primary	Approved	View
AIDS-related Kaposi's sarcoma	Primary	Approved	View
Multiple myeloma	Primary	Approved	View
Locally advanced or unresectable soft tissue sarcoma	Primary	Phase III	View
Kaposi's sarcoma	Primary	Phase II	View
Glioblastoma	Primary	Phase II	View
Lung non-small cell carcinoma			View
Pancreatic ductal adenocarcinoma			View

This label may not be the latest approved by FDA.
For current labeling information, please visit <https://www.fda.gov/drugsatfda>

HIGHLIGHTS OF PRESCRIBING INFORMATION
These highlights do not include all the information needed to use DOXIL safely and effectively. See full prescribing information for DOXIL.
DOXIL® (doxorubicin HCl liposome injection) for intravenous infusion
Initial U.S. Approval: 1995

WARNING: INFUSION REACTIONS, MYELOSUPPRESSION, CARDIOTOXICITY, LIVER IMPAIRMENT, SUBSTITUTION
See full prescribing information for complete boxed warning.

- Myocardial damage may lead to congestive heart failure and may occur as the total cumulative dose of doxorubicin HCl approaches 550 mg/m². Cardiac toxicity may also occur at lower cumulative doses with mediastinal irradiation or concurrent cardiotoxic agents (5.1).
- Acute infusion-related reactions, sometimes reversible upon terminating or slowing infusion, occurred in up to 10% of patients. Serious and sometimes fatal allergic/anaphylactoid-like infusion reactions have been reported. Medication/emergency equipment to treat such reactions should be available for immediate use (5.2).
- Severe myelosuppression may occur (5.3).
- Reduce dosage in patients with impaired hepatic function (2.6).
- Accidental substitution of DOXIL resulted in severe side effects. Do not substitute on mg per mg basis with doxorubicin HCl (2.1).

RECENT MAJOR CHANGES
Contraindications, Nursing Mothers (4) Removed 8/2013
Warnings and Precautions, Secondary Oral Neoplasms (5.5) 8/2013

INDICATIONS AND USAGE
DOXIL is an anthracycline topoisomerase inhibitor indicated for:

- Ovarian cancer (1.1)
- AIDS-related Kaposi's Sarcoma (1.2)
- After failure of prior systemic chemotherapy.
- Multiple Myeloma (1.3)

In combination with bortezomib in patients who have not previously received bortezomib and have received at least one prior therapy.

DOXIL can be used in combination with the following drugs:

DOSAGE AND ADMINISTRATION
Administer DOXIL as an initial rate of 1 mg/min to minimize the risk of infusion reactions. If no infusion related reactions occur, increase rate of infusion.

FULL PRESCRIBING INFORMATION: CONTENTS*
WARNING: INFUSION REACTIONS, MYELOSUPPRESSION, CARDIOTOXICITY, LIVER IMPAIRMENT, ACCIDENTAL SUBSTITUTION

1 INDICATIONS AND USAGE
1.1 Ovarian Cancer
1.2 AIDS-Related Kaposi's Sarcoma
1.3 Multiple Myeloma
2 DOSAGE AND ADMINISTRATION
2.1 Usage and Administration Precautions
2.2 Patients With Ovarian Cancer
2.3 Patients With AIDS-Related Kaposi's Sarcoma
2.4 Patients With Multiple Myeloma

6 ADVERSE REACTIONS
6.1 Overall Adverse Reactions Profile
6.2 Adverse Reactions in Clinical Trials
6.3 Post Marketing Experience
7 DRUG INTERACTIONS
8 USE IN SPECIFIC POPULATIONS
8.1 Pregnancy
8.3 Nursing Mothers
8.4 Pediatric Use
8.5 Geriatric Use
8.6 Hepatic Impairment
10 OVERDOSAGE
11 DESCRIPTION
12 CLINICAL PHARMACOLOGY

Infusion to complete administration over 1 hour. Do not administer as bolus injection or undiluted solution (2.1).

- Ovarian cancer: 50 mg/m² IV every 4 weeks for 4 courses minimum (2.2)
- AIDS-related Kaposi's Sarcoma: 20 mg/m² IV every 3 weeks (2.3)
- Multiple Myeloma: 30 mg/m² IV on day 4 following bortezomib which is administered at 1.3 mg/m² bolus on days 1, 4, 8 and 11, every 3 weeks (2.4)

DOSAGE FORMS AND STRENGTHS
Single use vial: 20 mg/10 mL and 50 mg/25mL (3)

CONTRAINDICATIONS
• Hypersensitivity reactions to a conventional formulation of doxorubicin HCl or the components of DOXIL (4, 5.5)

WARNINGS AND PRECAUTIONS
• Hand-Foot Syndrome may occur. Dose modification or discontinuation may be required (5.4)
• Radiation recall reaction may occur (5.5)

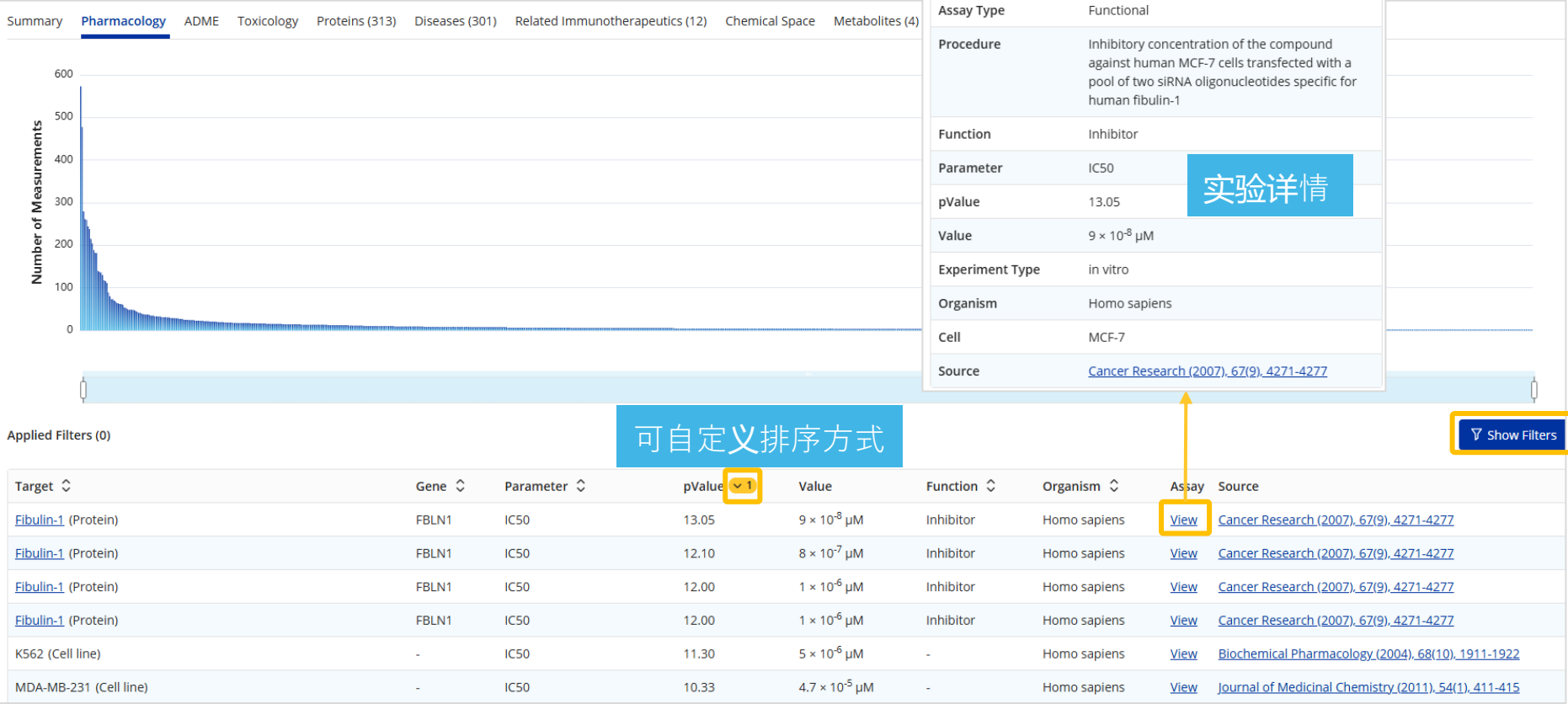
ADVERSE REACTIONS
Most common adverse reactions (≥20%) are asthenia, fatigue, fever, anorexia, nausea, vomiting, stomatitis, diarrhea, constipation, hand and foot syndrome, rash, neutropenia, thrombocytopenia and anemia (6).

To report SUSPECTED ADVERSE REACTIONS contact Janssen Products, LP at 1-800-JANSSEN (1-800-326-7736) or FDA at 1-800-FDA-1088 or www.fda.gov/medwatch.

DRUG INTERACTIONS
• DOXIL may formulations
• DOXIL can
• Discontinue

See 17 for PATIENT COUNSELING INFORMATION. Revised: 08/2013

配体药理学信息



← Prev (1 of 9,000) Next →

Target	Fibulin-1 (Protein)
Gene	FBLN1
Assay Type	Functional
Procedure	Inhibitory concentration of the compound against human MCF-7 cells transfected with a pool of two siRNA oligonucleotides specific for human fibulin-1
Function	Inhibitor
Parameter	IC50
pValue	13.05
Value	$9 \times 10^{-8} \mu\text{M}$
Experiment Type	in vitro
Organism	Homo sapiens
Cell	MCF-7
Source	Cancer Research (2007). 67(9). 4271-4277

实验详情

药理活性实验数据筛选项

Filters

Chemical Filters	
▼ pValue	
Biological Filters	
▼ Target	靶点
▼ Target Type	靶点类型
▼ Disease	疾病
▼ Organism	生物有机体
▼ Parameter	药理学参数
▼ Function	功能
▼ Experiment Type	实验类型
Source Filters	
▼ Document Type	
▼ Publication Year	
▼ Language	

Organism

- ☐ Homo sapiens
- ☐ Mus musculus
- ☐ H. EP.2 ATCC CCL23
- ☐ Rattus norvegicus
- ☐ Sus scrofa

[View All](#) Apply

Parameter

- ☐ IC50
- ☐ GI50
- ☐ Cell viability
- ☐ Inhibition
- ☐ Protein expression

[View All](#) Apply

Function

- ☐ Inhibitor
- ☐ Modulator
- ☐ Binder
- ☐ Substrate
- ☐ Antagonist

[View All](#) Apply

配体ADME信息

Summary Pharmacology **ADME** Toxicology Proteins (313) Diseases (301) Related Immunotherapeutics (12) Chemical Space Metabolites (4) Similar Ligands (764)

Predicted Properties

logP* - Partition Coefficient0.918

logS - Solubility-3.27

logBB - Blood-Brain Barrier Permeability-1.96

Polar surface area (Å²)*206.07

Plasma protein binding67.32

Permeability glycoprotein1

* Calculated using Advanced Chemistry Development Software (© 1994-2025 ACD/Labs)

Applied Filters (0)

Parameter ^ 1	Value	Organism ^	Assay	Source
t1/2	9.63 hr	Rattus	View	International Journal of Pharmaceutics (Amsterdam, Netherlands)(2019), 557(1), 264-272
t1/2	32 hr	Rattus	View	Journal of Pharmaceutical Sciences (St. Louis, MO)(2019), 108(1), 1100-1101
t1/2	6.8 hr	Macaca mulatta	View	Anticancer Research (Tampa, FL)(2019), 39(1), 2004385
t1/2	5.7 hr	Mus	View	Advanced Drug Delivery Reviews (Amsterdam, Netherlands)(2019), 148, 106824 A1 2013-07-18
t1/2	11.9 hr	Mus musculus	View	World Journal of Pharmaceutical Research (Deemed to be University, Hyderabad, India)(2023), 12(1), 273-285
t1/2	17.9 hr	Rattus	View	International Journal of Pharmaceutics (Amsterdam, Netherlands)(2017), 526(1-2), 443-454
t1/2	3.5 hr		View	Biochemical Pharmacology (New York, NY)(2017), 101, 4279-4288
t1/2	0.8 hr		View	AAI (Amsterdam, Netherlands)(2017), 526(1-2), 443-454
t1/2	15.9 hr		View	Anticancer Research (Tampa, FL)(2017), 37(1), 4279-4288
Vd	970.8667 L		View	International Journal of Pharmaceutics (Amsterdam, Netherlands)(2017), 526(1-2), 443-454

← Prev (641 of 732) Next →

Assay Name	Half-life measurement
Assay Type	Functional
Route of Administration	Intravenous
Procedure	Half life determined
Parameter	t1/2
Value	9.63 hr
Experiment Type	in vivo
Organism	Rattus
Organism Detail	Sprague-dawley
Source	International Journal of Pharmaceutics (Amsterdam, Netherlands)(2019), 557(1), 264-272

实验详情

ADME实验数据筛选项

Filters

Biological Filters

Organism

☐ Mus

☐ Rattus

☐ Homo sapiens

☐ Rattus norvegicus

☐ Macaca mulatta

生物有机体

Show Filters

Apply

Parameter

☐ t1/2

☐ Cmax

☐ AUC

☐ CL

☐ Vd

代谢相关参数

View All

Apply

Experiment Type

☐ in vivo

☐ in vitro

实验类型

View All

Apply

Source Filters

Document Type

Publication Year

Language

配体毒理学信息

Parameter	Value	Organism	Assay	Source
ED (effective dose)	3.16228 × 10 ⁴ μM	Mus musculus	View	Journal of Medicinal Chemistry (2003), 46(14), 2985-3007
IC10	0.2 μM	Mus musculus	View	TIVIEQ Toxicology In Vitro. (Pergamon Press Inc., Maxwell House, Fairview Park, Elmsford, NY 10523) V.1- 1987- Volume(issue)/page/year
IC10	0.012 μM	Homo sapiens	View	TXAPA9 Toxicology and Applied Pharmacology. (Academic Press, Inc., 1 E. First St., Duluth, MN 55802) V.1- 1959- Volume(issue)/page/year
IC10	0.06 μM	Mus musculus	View	TIVIEQ Toxicology In Vitro. (Pergamon Press Inc., Maxwell House, Fairview Park, Elmsford, NY 10523) V.1- 1987- Volume(issue)/page/year
IC20	0.022 μM	Homo sapiens	View	TXAPA9 Toxicology and Applied Pharmacology. (Academic Press, Inc., 1 E. First St., Duluth, MN 55802) V.1- 1959- Volume(issue)/page/year
IC50	0.08 μM	Homo sapiens	View	AMCLCT ACS Medicinal Chemistry Letters. (American Chemical Society, 1155 Sixteenth Street N.W., Washington, DC 20036) V.1- 2010- Volume(issue)/page/year
IC50	0.48 μM	Homo sapiens	View	AMCLCT ACS Medicinal Chemistry Letters. (American Chemical Society, 1155 Sixteenth Street N.W., Washington, DC 20036) V.1- 2010- Volume(issue)/page/year
IC50	0.14 μM	Homo sapiens	View	TIVIEQ Toxicology In Vitro. (Pergamon Press Inc., Maxwell House, Fairview Park, Elmsford, NY 10523) V.1- 1987- Volume(issue)/page/year
IC50	1 mg/L	Homo sapiens	View	FRM
IC50	4.8 mg/L	Mus musculus	View	JOET

Assay Type

Functional

Procedure

Log cell kill of tumor bearing mice was determined by the dose of 162 mg/K

Assay Type	Functional
Procedure	Log cell kill of tumor bearing mice was determined by the dose of 162 mg/K
Parameter	ED (effective dose)
Parameter Detail	Log Kill
pValue	1.50
Value	$3.16228 \times 10^4 \mu\text{M}$
Disease	Cancer
Experiment Type	in vivo
Organism	Mus musculus
Source	Journal of Medicinal Chemistry (2003), 46(14), 2985-3007

[illegible]

配体相关靶点与疾病信息

基于CAS数据关联，一键关联到该配体相关靶点与疾病信息详情页，并探索更多关联信息

Doxorubicin

CAS Registry Number: 23214-92-8

112K

1,642

Retrosynthesis

Predictive Analytics

⋮

SummaryPharmacologyADMEToxicologyProteins (313)Diseases (301)Related Immunotherapeutics (12)Chemical SpaceMetabolites (4)Similar Ligands (764)

View: ListSort: RelevanceView all associated proteins

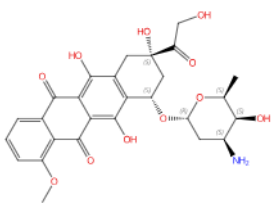
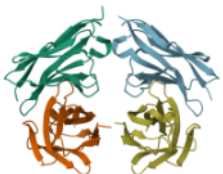
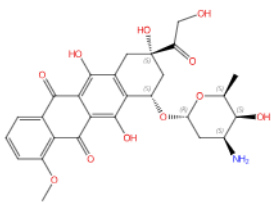
Protein	Organism
1 KDR Vascular endothelial growth factor receptor 2	-
2 EGFR Epidermal growth factor receptor	-
3 KDR Vascular endothelial growth factor receptor 2	Homo sapiens
4 SRC Proto-oncogene tyrosine-protein kinase Src	-
5 CYP3A4 Cytochrome P450 3A4	Homo sapiens

DiseasesAdverse Events副作用

Sort: RelevanceView all associated diseases

Disease	Description	Biomarkers
1 Cancer	A disease of cellular proliferation that is malignant and primary, characterized by uncontrolled cellular proliferation, local cell invasion and metastasis.	BRCA1 DNA repair associated, Neurotrophin 4, Autophagy related 16 like 1, Major histocompatibility complex, class II, DP beta 1, KRAS proto-oncogene, GTPase, View All
2 Alzheimer's disease	A tauopathy that is characterized by memory lapses, confusion, emotional instability and progressive loss of mental ability and results in progressive memory loss, impaired thinking, disorientation, and changes in personality and mood starting and leads in advanced cases to a profound decline in cognitive and physical functioning and is marked histologically by the degeneration of brain neurons especially in the cerebral cortex and by the presence of neurofibrillary tangles and plaques containing beta-amyloid.	Apolipoprotein E, Fibrinogen alpha chain, Islet amyloid polypeptide, APP (rs199862130) polymorphism, Synuclein alpha, View All
3 Rheumatoid arthritis	An arthritis that is an autoimmune disease which attacks healthy cells and tissue located in joint.	TIMP metalloproteinase inhibitor 1, Solute carrier family 22 member 4, Tumor necrosis factor, Matrix metalloproteinase 1, Protein kinase C theta, View All
4 Asthma	A bronchial disease that is characterized by chronic inflammation and narrowing of the airways, which is caused by a combination of environmental and genetic factors. The disease has symptom recurring periods of wheezing (a whistling sound while breathing), has symptom chest tightness, has symptom shortness of breath, has symptom mucus production and has symptom coughing.	Membrane spanning 4-domains A2, Transient receptor potential cation channel subfamily A member 1, Adrenomedullin, Fc epsilon receptor 1a, CDKN2B-AS1 (rs7859362) polymorphism, View All
5 Diabetes mellitus	A glucose metabolism disease that is characterized by chronic hyperglycaemia with disturbances of carbohydrate, fat and protein metabolism resulting from defects in insulin secretion, insulin action, or both.	MTHFR (rs1801133) polymorphism, Cytokine inducible SH2 containing protein, Cystatin C, Insulin, Mechanistic target of rapamycin kinase, View All
6 Bacterial infectious disease	A disease by infectious agent that results in infection, has material basis in Bacteria.	Tumor necrosis factor, Activation induced cytidine deaminase, Serum amyloid A1, Transforming growth factor beta 1, C-C motif chemokine ligand 17, View All

配体相关免疫疗法信息

Summary Pharmacology ADME Toxicology Proteins (313) Diseases (301) Related Immunotherapeutics (12) Chemical Space Metabolites (4) Similar Ligands (764)															
MAb-DMBA-SIL-Dox   Absolute stereochemistry shown 抗体与配体结构信息	<table><tr><td>Antibody</td><td>Cetuximab</td></tr><tr><td>Antigen</td><td>Epidermal growth factor receptor (EGFR)</td></tr><tr><td>Payload</td><td>Doxorubicin</td></tr><tr><td>Therapeutic Target</td><td>DNA topoisomerase 2-alpha</td></tr><tr><td>Drug-Antibody Ratio</td><td>5.57</td></tr><tr><td>Linker</td><td>DMBA-SIL</td></tr><tr><td>Method</td><td>Site-specific conjugation with the respective EGFR mAb via thiolmaleimide Michael addition.</td></tr></table>	Antibody	Cetuximab	Antigen	Epidermal growth factor receptor (EGFR)	Payload	Doxorubicin	Therapeutic Target	DNA topoisomerase 2-alpha	Drug-Antibody Ratio	5.57	Linker	DMBA-SIL	Method	Site-specific conjugation with the respective EGFR mAb via thiolmaleimide Michael addition.
Antibody	Cetuximab														
Antigen	Epidermal growth factor receptor (EGFR)														
Payload	Doxorubicin														
Therapeutic Target	DNA topoisomerase 2-alpha														
Drug-Antibody Ratio	5.57														
Linker	DMBA-SIL														
Method	Site-specific conjugation with the respective EGFR mAb via thiolmaleimide Michael addition.														
Trastuzumab-PC4AP-DOX   Absolute stereochemistry shown 抗体与配体结构信息	<table><tr><td>Antibody</td><td>Trastuzumab</td></tr><tr><td>Antigen</td><td>Receptor tyrosine-protein kinase erbB-2 (ERBB2)</td></tr><tr><td>Payload</td><td>Doxorubicin</td></tr><tr><td>Therapeutic Target</td><td>DNA topoisomerase 2-alpha</td></tr><tr><td>Drug-Antibody Ratio</td><td>2</td></tr><tr><td>Linker</td><td>Photocaged C4AP</td></tr><tr><td>Method</td><td>Random conjugation through reduced inter-chain cysteines.</td></tr></table>	Antibody	Trastuzumab	Antigen	Receptor tyrosine-protein kinase erbB-2 (ERBB2)	Payload	Doxorubicin	Therapeutic Target	DNA topoisomerase 2-alpha	Drug-Antibody Ratio	2	Linker	Photocaged C4AP	Method	Random conjugation through reduced inter-chain cysteines.
Antibody	Trastuzumab														
Antigen	Receptor tyrosine-protein kinase erbB-2 (ERBB2)														
Payload	Doxorubicin														
Therapeutic Target	DNA topoisomerase 2-alpha														
Drug-Antibody Ratio	2														
Linker	Photocaged C4AP														
Method	Random conjugation through reduced inter-chain cysteines.														

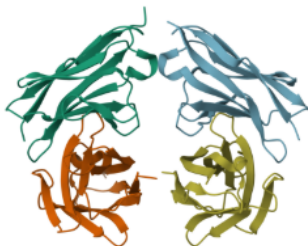
ADC药物详情页

Trastuzumab emtansine

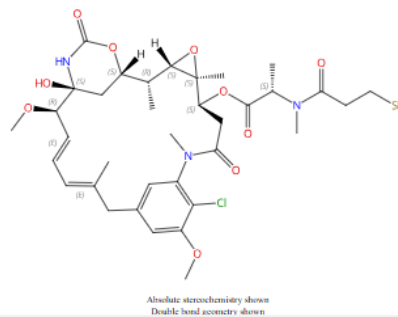
CAS Registry Number: 1018448-65-1

1,972 8 Retrosynthesis Predictive Analytics

Summary Pharmacology ADME Proteins (2) Diseases (1)



抗体3D结构图



药物分子结构

CAS DRUG INTELLIGENCE

药物情报信息

Approved Drug

Trastuzumab emtansine (ado-trastuzumab emtansine, trade name Kadcyla) is a combination between a monoclonal antibody and a small-molecule drug. Each molecule of trastuzumab emtansine consists of a single trastuzumab molecule with several molecules of DM1, a cytotoxic maytansinoid, attached. SMCC, or...

View More

STATUS	Approval Status: US Approved Approval Authority: US FDA Approval Year: 2013 Originator: Genentech
INDICATIONS	Breast cancer Modality: Primary Highest Phase: Approved Source
PRIMARY TARGET	Receptor tyrosine-protein kinase erbB-2 Function: Blocker Source

Antibody	Trastuzumab
Antigen	Receptor tyrosine-protein kinase erbB-2 (ERBB2)
Payload	Mertansine DM1
Therapeutic Target	Microtubule
Drug-Antibody Ratio	3.5
Linker	Succinimidyl-4-(N-maleimidomethyl)cyclohexane-1-carboxylate (SMCC)
Method	Random conjugation through nucleophilic lysines.

ADC药物详情

Heavy Chain Sequence

EVQLVESGGGLVQPGGSLRLSCAASG**GFNIKDTY**IHWVRQAPGKGLEWVAR**IYPTNGYT**TRYADSVKGRFTISADTSKNTAYLQMNSLRAEDTAVYY**SRWGGDG**
FYAMDYDYWGQGLVTVSSASTKGPSVFPLAPSSKSTSGGTAALGCLVKDYFPEPTVTSWNSGALTSGVHTFPAVLQSSGLYSLSSVTPVSSSLGTQTYICNV
NHKPSNTKVDKKVEPKSCDKTHTCPPCPAPELLGGPSVFLFPPKPKDTLMISRTPEVTCVVDVSHEDPEVKFNWYVDGVEVHNAKTKPREEQYNSTYRVVSVL
TVLHQDWLNGKEYKCKVSNKALPAPIEKTISKAKGQPREPQVYTLPPSREEMTKNQVSLTCLVKGFYPSDIAVEWESNGQPENNYKTPPVLDSDGSFFLYSKL
TVDKSRWQQGNVFCSCVMHEALHNHYTQKSLSLSPGK

重链/轻链序列

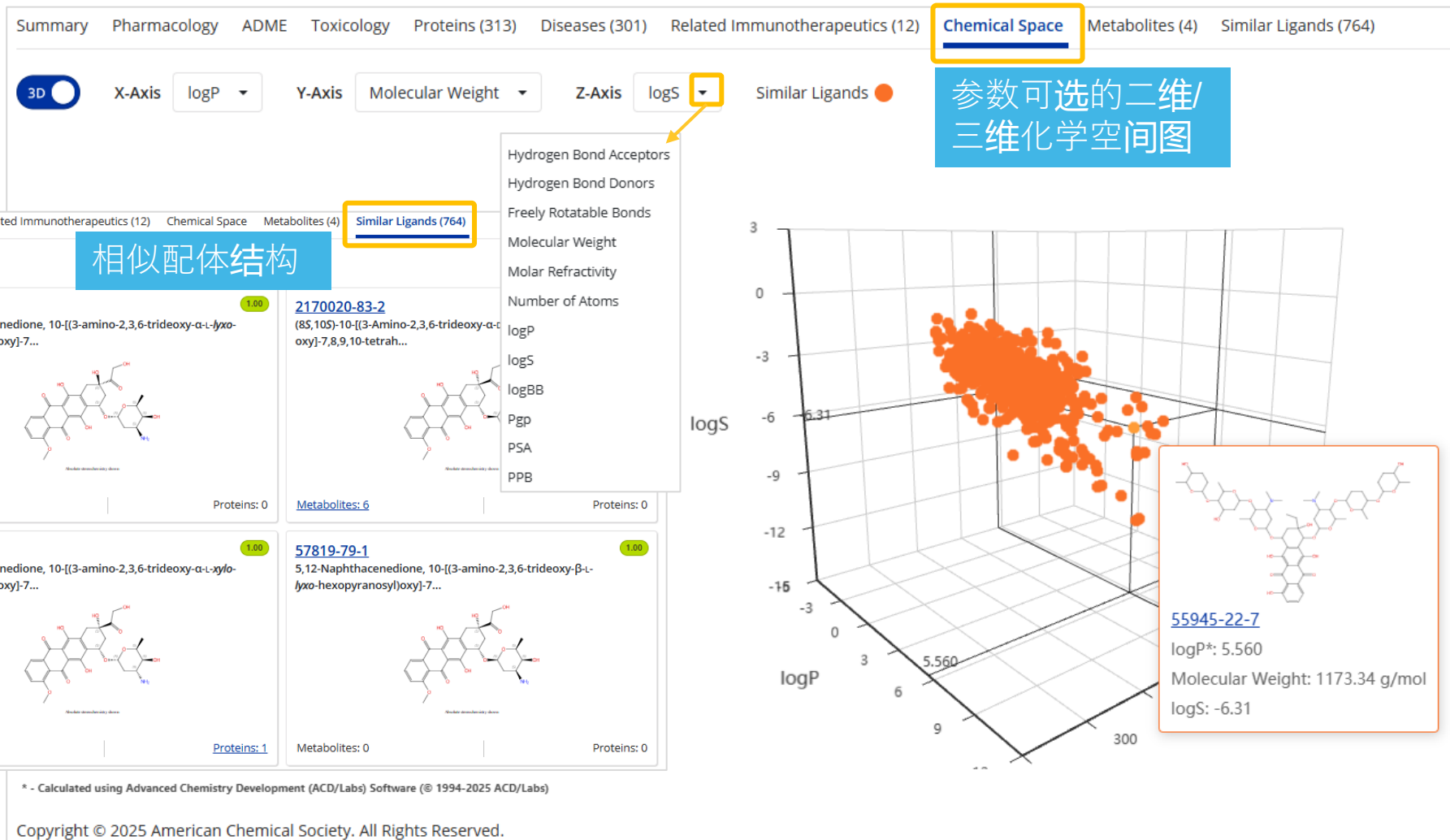
Light Chain Sequence

DIQMTQSPSSLS**SAS**VGDRVTITCRAS**QDVNTA**AVAWYQQKPGKAPKLLIYSASFLYSGVPSRFSGSRSGTDFTLTISLQPEDFATYY**QQHYTTPPT**PTFGQG
TKVEIKRTVAAPSVFIFPPSDEQLKSGTASVVCLLNNFYPREAKVQWKVDNALQSGNSQESVTEQDSKDSYSTLSSTLTLSKADYEKHKVYACEVTHQGLSSPV
TKSFNRGEC

HCDR1 GFNIKDTY	HCDR2 IYPTNGYT	HCDR3 SRWGGDGFYAMDY	LCDR2 SAS	LCDR1 QDVNTA	LCDR3 QQHYTTPPT
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CDR序列

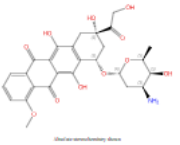
相似配体结构与可视化分析



探索配体代谢产物

已知代谢产物：Known

预测代谢产物：Confidence Score置信度分值，
表示发生该生物转化的概率

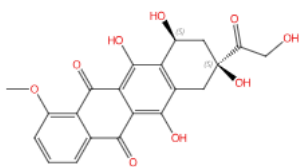


Doxorubicin
CAS Registry Number: 23214-92-8

112K 1,642 Retrosynthesis Predictive Analytics

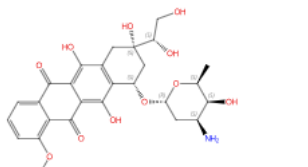
Summary Pharmacology ADME Toxicology Proteins (313) Diseases (301) Related Immunotherapeutics (12) Chemical Space **Metabolites (4)** Similar Ligands (764)

24385-10-2 Known



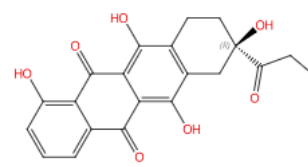
Absolute stereochemistry shown

54193-28-1 Known



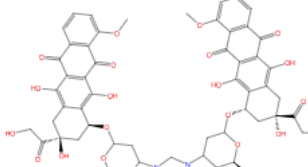
Absolute stereochemistry shown

69417-09-0 Known



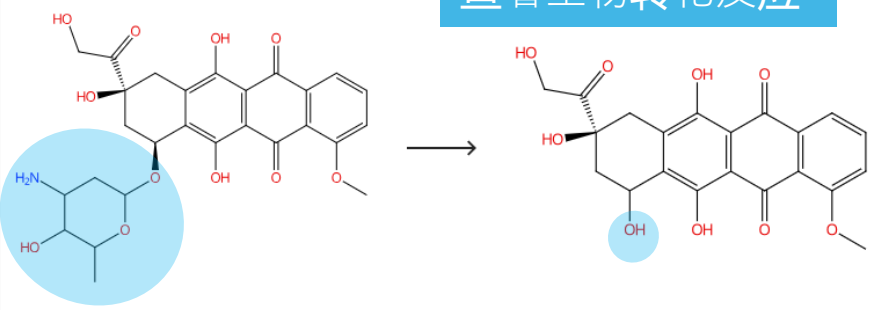
Absolute stereochemistry shown

Known



Transformation of 23214-92-8 to 24385-10-2

查看生物转化反应



Facilitator	Organism	Source
-	Homo sapiens	Chemical Research in Toxicology (2000), 13(5), 414-420

提纲

- CAS BioFinder 简介与检索界面介绍 (Introduction and Interface)
- 配体检索与配体详情信息 (Ligands and Details Overview)
- 骨架检索与构效关系分析 (Scaffolds and SAR Analysis)
- 蛋白/通路/靶点、疾病与生物标志物 (Proteins & Pathways; Diseases & Biomarkers)
- 生物活性预测 (Predictive Analytics)

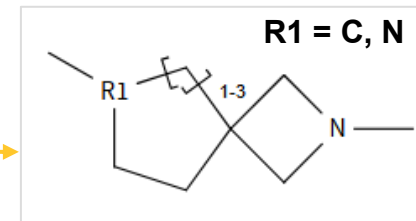
基于靶点或结构片段，探索活性结构骨架

[Ligands](#)
[Scaffolds](#)
[Proteins](#)
[Diseases](#)

Search by disease name, ligand, protein, or draw a structure.

绘制核心结构片段

Draw a Structure



Filters

Chemical Filters

Rule of 5 Filter Preset ☐ OFF This will automatically be applied.

^ pValue
1.70 to 13.00

Reset Filter

Modality

Druglikeness

ADME

Commercial Availability

Approval Status

Approval Authority

Biological Filters

Target

- ☐ Menin
- ☐ Cyclin E1-CDK2 complex
- ☐ Histone-lysine N-methyltransferase complex
- ☐ GTPase KRas
- ☐ Monoglyceride lipase

[View All](#)

Scaffolds search for drawn structure

Ligands Scaffolds Pharmacology

2,649 Results

1
Ligands: 210 Proteins: 9

2
Ligands: 11 Proteins: 5

3
Ligands: 55 Proteins: 1

4
Ligands: 20 Proteins: 4

5
Ligands: 34 Proteins: 1

6
Ligands: 12 Proteins: 3

7
Ligands: 8 Proteins: 12

8
Ligands: 31 Proteins: 1

10
Ligands: 8 Proteins: 12

11
Ligands: 8 Proteins: 12

12
Ligands: 8 Proteins: 12

归一化的活性

筛选关注的靶点

$$pKa = -\log_{10} Ka$$

$$pIC50 = -\log_{10} IC50$$

IC50越小，
pValue越大，
抑制活性越高。

探索目标结构骨架的SAR数据



Scaffolds

Search by protein, ligand, disease or draw a structure.

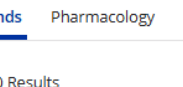


 Edit



[Return to Results](#)

Scaffold Summary



Associated Proteins
1

Filters

Chemical Filters ▲

☐ Rule of 5 Filter Preset
This will automatically be applied.

▼ R-Groups

▼ pValue

▼ Druglikeness

▼ ADME

▼ Commercial Availability

Biological Filters ▲

▼ Target

▼ Target Type

▼ Disease



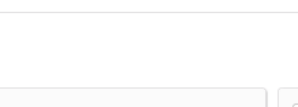
GIELXZVQJYHYPI-UHFFFAOYSA-N
 Murcko scaffold InChI Key

Ligands

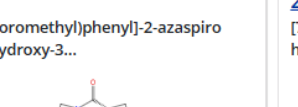
Pharmacology

Similar Scaffolds

☐ 60 Results

☐ 1
[2765314-82-5](#)
 [7-(2,5-Difluoro-3-methoxyphenyl)-2-azaspiro[3.5]non-2-yl](*cis*-3-hydroxy-3-methy...

Relative stereochemistry shown

[Metabolites: 4](#)
[Proteins: 1](#)

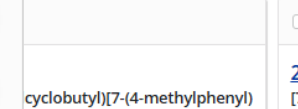
☐ 2
[2765312-35-2](#)
 [7-[3-Ethoxy-5-(trifluoromethyl)phenyl]-2-azaspiro[3.5]non-2-yl](*cis*-3-hydroxy-3...

Relative stereochemistry shown

[Metabolites: 4](#)
[Proteins: 1](#)

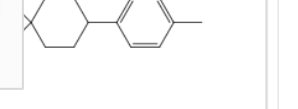
☐ 3
[2765312-62-5](#)
 [7-(3,5-Dimethylphenyl)-2-azaspiro[3.5]non-2-yl](*cis*-3-hydroxy-3-methylcyclobutyl...

Relative stereochemistry shown

[Metabolites: 4](#)
[Proteins: 1](#)

☐ 4
[2765312-53-4](#)
 (*cis*-3-Hydroxy-3-methylcyclobutyl)[7-(2-methylphenyl)-2-azaspiro[3.5]non-2-yl]me...

Relative stereochemistry shown

[Metabolites: 7](#)
[Proteins: 1](#)

☐ 5
[2765312-61-4](#)
 [7-[3-Ethyl-5-(trifluoromethyl)phenyl]-2-azaspiro[3.5]non-2-yl](*cis*-3-hydroxy-3-methylcyclobutyl)[7-(4-methylphenyl)]me...

Relative stereochemistry shown

[Metabolites: 6](#)
[Proteins: 1](#)

☐ 7
[2765314-60-9](#)
 [7-(3,5-Dimethylphenyl)-7-methoxy-2-azaspiro[3.5]non-2-yl](*cis*-3-hydroxy-3-methy...

Relative stereochemistry shown

[Metabolites: 6](#)
[Proteins: 1](#)

☐ 8
[2765314-68-7](#)
 [7-(2-Fluoro-3-methylphenyl)-2-azaspiro[3.5]non-2-yl](*cis*-3-hydroxy-3-methylcyclobutyl)me...

Relative stereochemistry shown

[Metabolites: 5](#)
[Proteins: 1](#)



[Ligands: 60](#)
[Proteins: 1](#)

Sort: Relevance ▼  Get MMPA

R-Groups

R1 7

R2 13

R3 8

R4 5

R5 3

R8 1

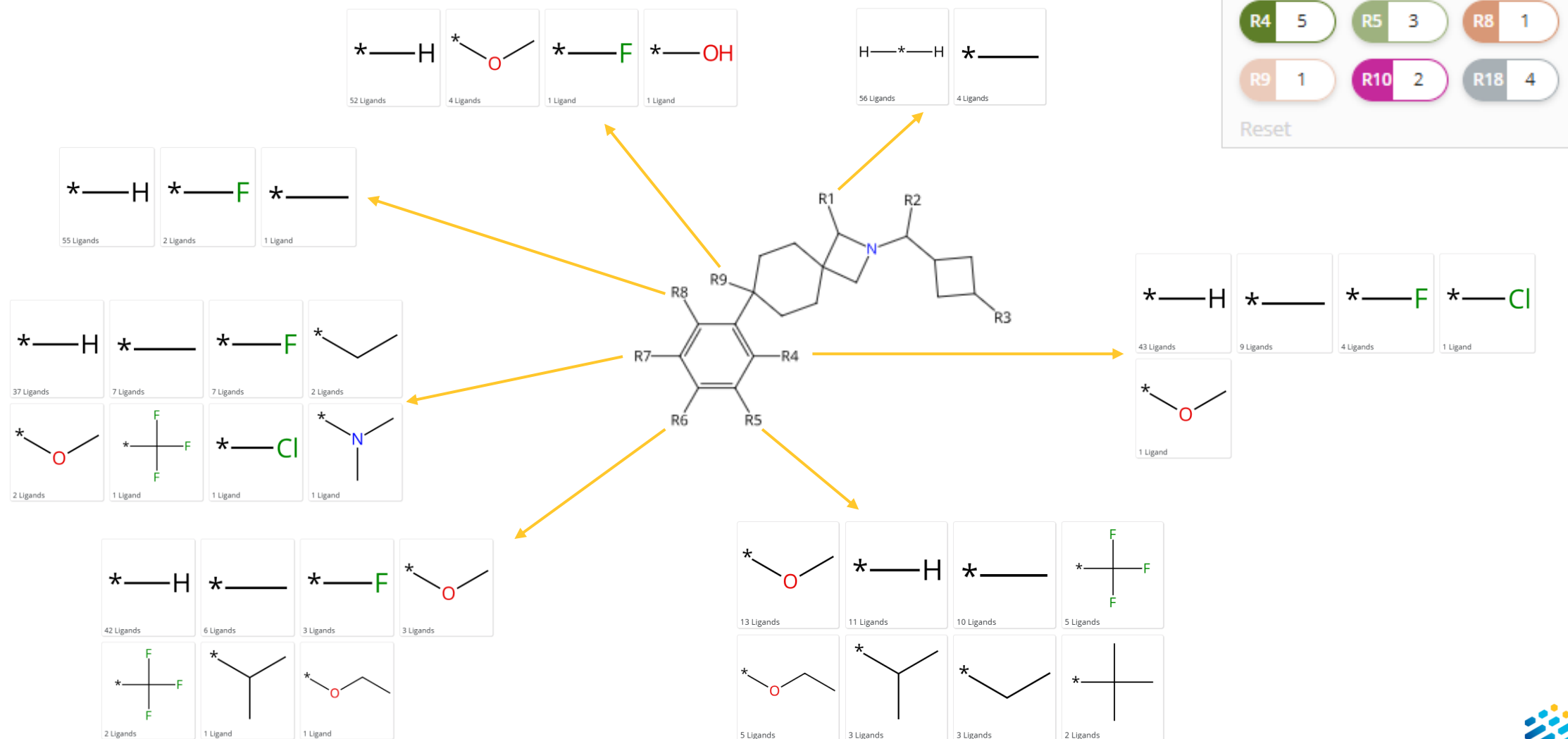
R9 1

R10 2

R18 4

Reset

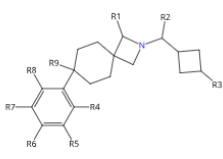
探索目标结构骨架的SAR数据



匹配分子对分析 (MMPA)

← [Return to Results](#)

Scaffold Summary



Associated Proteins
1

Filters

Chemical Filters

Rule of 5 Filter
OFF This will automatically filter out molecules that do not meet the Rule of 5 criteria.

^ R-Groups

GIELXZVQJYHYPI-UHFFFAOYSA-N
Murcko scaffold InChI Key

Ligands Pharmacology Similar Scaffolds

60 Results

Sort: Relevance [Get MMPA](#)

1 [2765314-82-5](#)
[7-(2,5-Difluoro-3-methoxyphenyl)-2-azaspiro[3.5]non-2-yl](cis-3-hydroxy-3-methy...

2 [2765312-35-2](#)
[7-[3-Ethoxy-5-(trifluoromethyl)phenyl]-2-azaspiro[3.5]non-2-yl](cis-3-hydroxy-3-methy...

3 [2765312-62-5](#)
[7-(3,5-Dimethylphenyl)-2-azaspiro[3.5]non-2-yl](cis-3-hydroxy-3-methylcyclobuty...

4 [2765312-53-4](#)
(cis-3-Hydroxy-3-methylcyclobutyl)[7-(2-methylphenyl)-2-azaspiro[3.5]non-2-yl]me...

Select a Target for Matched Molecular Pairs Analysis (MMPA)

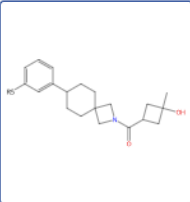
Target

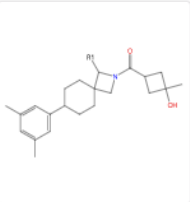
☒ Monoglyceride lipase

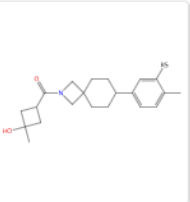
选择目标靶点

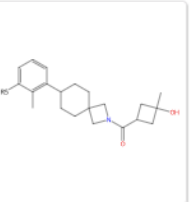
Next Cancel

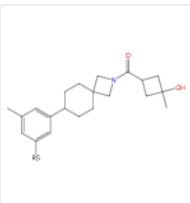
Select one R-Group Cluster to Visualize

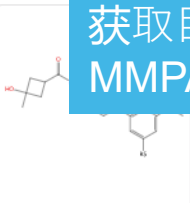

15 Matched Molecular Pairs

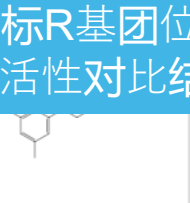

10 Matched Molecular Pairs


10 Matched Molecular Pairs


10 Matched Molecular Pairs


10 Matched Molecular Pairs


10 Matched Molecular Pairs


10 Matched Molecular Pairs


10 Matched Molecular Pairs

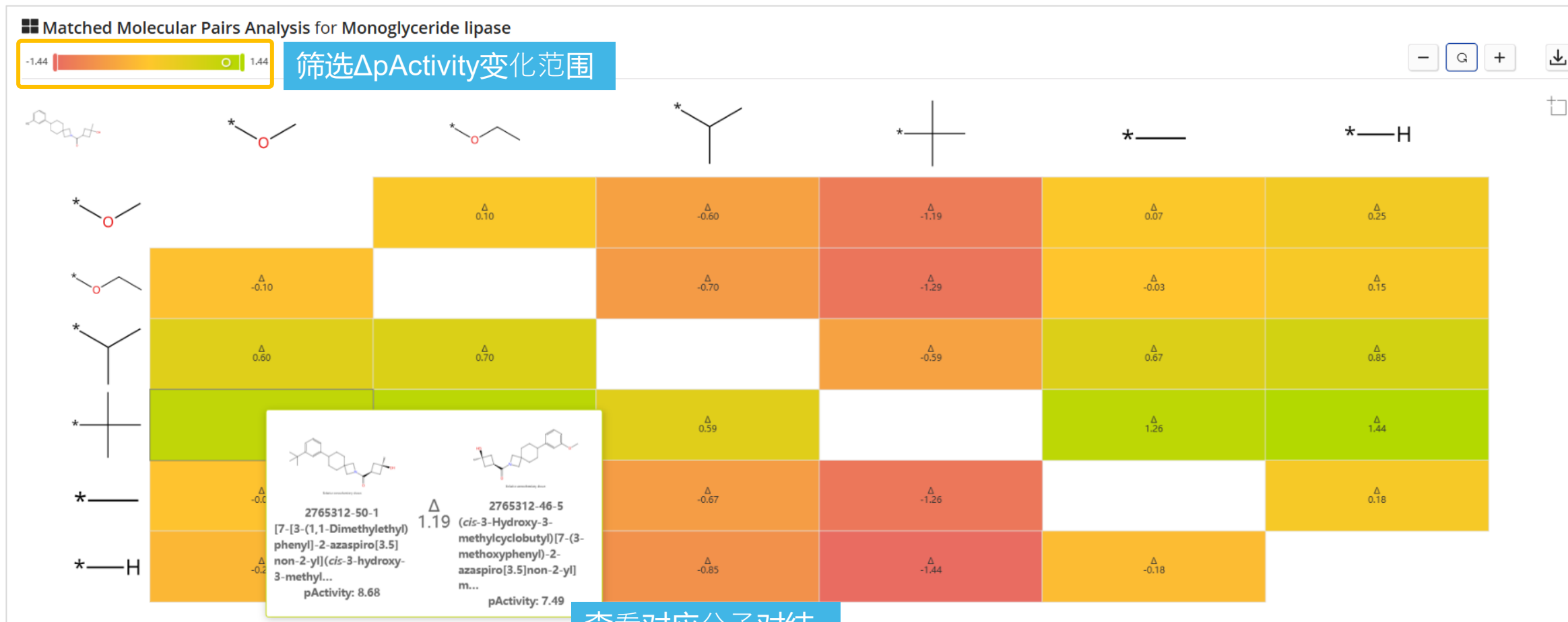
获取目标R基团位点变化的MMPA活性对比结果

Show 100 per page

Previous Submit Cancel

匹配分子对分析 (MMPA)

快速直观获取匹配分子对 $\Delta pActivity$ 热图



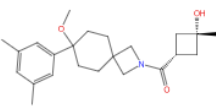
查看对应分子对结构信息与pActivity

查看同一结构骨架中的配体药理活性

Assay Detail

← Prev (1 of 60) Next →

Ligand
[2765314-60-9](#)


Relative stereochemistry shown

C₂₃H₃₃NO₃
[7-(3,5-Dimethylphenyl)-7-methoxy-2-azaspiro[3.5]non-2-yl][cis-3-hydroxy-3-methoxy-3-methylcyclobutyl]methanone

实验详情

Target	Monoglyceride lipase (Protein)
Gene	MGLL
Assay Type	Functional
Procedure	FAAH assay
Parameter	IC50
pValue	9.08
Value	8.4 × 10 ⁻⁴ μM
Disease	Disease of cellular proliferation
Experiment Type	in vitro
Organism	Homo sapiens
Cell	HeLa
Cell Detail	Cervical cancer cell
Source	United States_US20220089538 A1 2022-03-24

Scaffold Summary

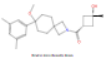
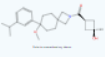
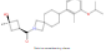
GIELXZVQJYHYPI-UHFFFAOYSA-N
Murcko scaffold InChI Key

Ligands **Pharmacology** Similar Scaffolds

Number of Measurements

Applied Filters (1) Target: Monoglyceride lipase X Clear all filters

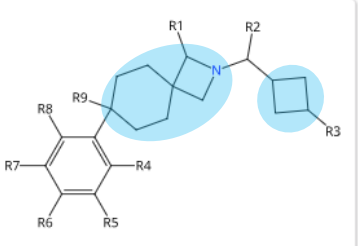
Show Structures **ON**

Ligand	Target	Gene	Parameter	pValue	Value	Function	Assay	Source
 2765314-60-9 [7-(3,5-Dimethylphenyl)-7-methoxy-2-azaspiro[3.5]non-2-yl][cis-3-hydroxy-3-methoxy-3-methylcyclobutyl]methanone	Monoglyceride lipase (Protein)	MGLL	IC50	9.08	8.4 × 10 ⁻⁴ μM	-	View	United States_US20220089538 A1 2022-03-24
 2765313-81-1 (cis-3-Hydroxy-3-methylcyclobutyl)[7-methoxy-7-[3-(1-methylethyl)phenyl]-2-azaspiro[3.5]non-2-yl]methanone	Monoglyceride lipase (Protein)	MGLL	IC50	8.92	0.0012 μM	-	View	United States_US20220089538 A1 2022-03-24
 2765314-75-6 (cis-3-Hydroxy-3-methylcyclobutyl)[7-[2-methyl-3-(1-methylethoxy)phenyl]-2-azaspiro[3.5]non-2-yl]methanone	Monoglyceride lipase (Protein)	MGLL	IC50	8.82	0.0015 μM	-	View	United States_US20220089538 A1 2022-03-24

筛选关注靶点

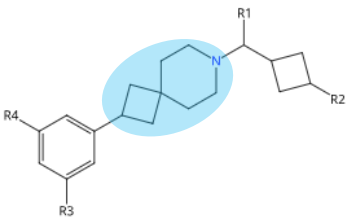
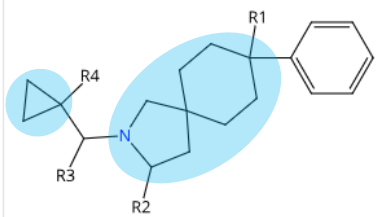
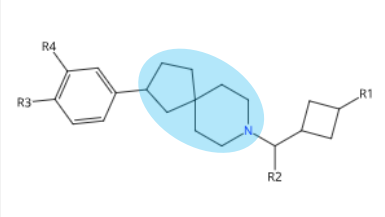
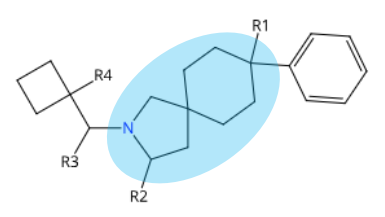
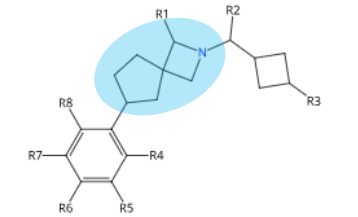
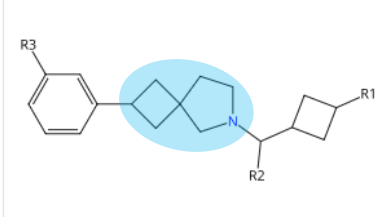
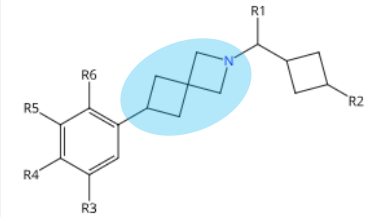
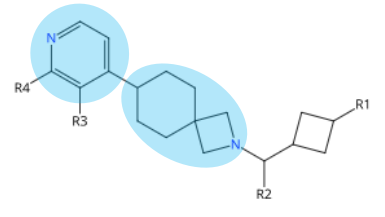
药理活性数据

获取与目标骨架相似骨架结构，启发新的SAR假设

[Return to Results](#)
Scaffold Summary

Associated Proteins
1

GIELXZVQJYHYPI-UHFFFAOYSA-N
Murcko scaffold InChI Key
Ligands Pharmacology **Similar Scaffolds**
1,123 Scaffolds

获取相似骨架结构 (Similar Scaffolds) ;
基于相应药效团的关键结构元素识别相似骨架结构

1  Ligands: 2 Proteins: 1	2  Ligands: 9 Proteins: 2	3  Ligands: 3 Proteins: 1	4  Ligands: 9 Proteins: 2
5  Ligands: 69 Proteins: 1	6  Ligands: 1 Proteins: 1	7  Ligands: 9 Proteins: 1	8  Ligands: 2 Proteins: 1

提纲

- CAS BioFinder 简介与检索界面介绍 (Introduction and Interface)
- 配体检索与配体详情信息 (Ligands and Details Overview)
- 骨架检索与构效关系分析 (Scaffolds and SAR Analysis)
- 蛋白/通路/靶点、疾病与生物标志物 (Proteins & Pathways; Diseases & Biomarkers)
- 生物活性预测 (Predictive Analytics)

通过靶点、疾病或配体， 获取归一化的蛋白检索结果

CAS BioFinder

Proteins SYK 示例：SYK

Filters

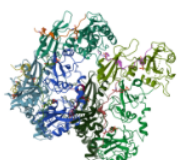
- Chemical Filters
- Biological Filters
 - Protein
 - Disease
 - Organism
 - Parameter
 - Function
 - Experiment Type
- Source Filters
 - Document Type
 - Publication Year
 - Language

Proteins search for SYK

Proteins Pharmacology

4 Results

Sort: Relevance View: **Grid** / List

1 SYK (Homo sapiens) Tyrosine-protein kinase SYK  Diseases: 223 Ligands: 17K	2 SYK Tyrosine-protein kinase SYK  Diseases: 344 Ligands: 16K	3 Syk (Rattus norvegicus) Tyrosine-protein kinase SYK  Diseases: 15 Ligands: 546	4 Syk (Mus musculus) Tyrosine-protein kinase SYK  Diseases: 13 Ligands: 35
--	---	--	--

切换缩略图视图
或列表视图

[Return to top](#)

蛋白详情信息与立体结构展示

SYK

Tyrosine-protein kinase SYK

Summary

Pharmacology

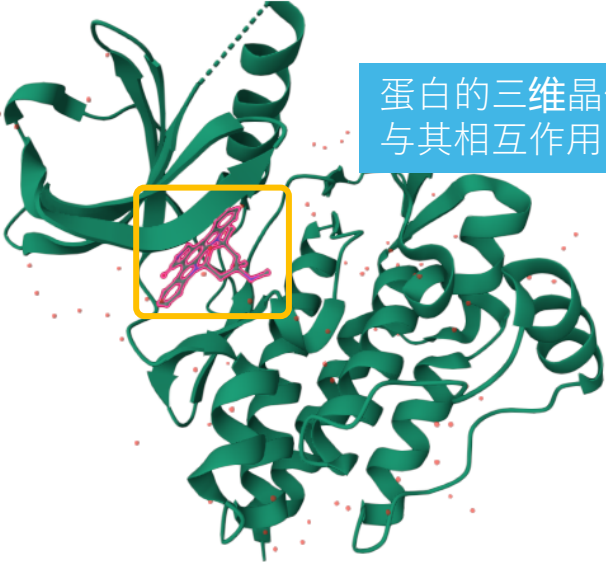
Ligands (31K)

Diseases (388)

Chemical Space

Pathways

Crystal structure of the syk tyrosine kinase domain with Staurosporin



蛋白的三维晶体结构及与其相互作用的小分子

STAUROSPORINE

1XBC | Model 1 | Instance ASML1 | B [auth A] | STU 1

1XBC

↺

+

-

↓

下载cif格式结构文件

Homo sapiens

unspecified

Rattus norvegicus

Mus musculus

来源有机体

Organism

Homo sapiens

GET FASTA

Copy Sequence

>P43405-1|Tyrosine-protein kinase SYK|Homo sapiens

MASSGMADSANHLPFFFGNITREEAEDYLQGGMSDGLYLLRQSRNYLGGFALSVAHGRKAHHTIERELNGTYAAGGRTHASPADLCHYHSQESDGLVCLLKKPFNRPQGVQPK

TGPFEDLKENLIREYVKQTWNLQGQALEQAIISQKPQLEKIATTAHEKMPWFHGKISRSESEQIVLIGSKTNGKFLIRARDNNGSYALCLLHEGKVLHYRIDKDTGKLSIPEGK

KFDTLWQLVEHYSYKADGLLRVLTPCQKIGTQGNVNFGGRPQLPGSHPATWSAGGISRIKSYSFPPKPGHRKSSPAQGNRQESTVSFNPEPELAPWAADKGPQREALPMDTEVY

ESPYADPEEIRPKEVYLDRKLLTLEDKELGSGNFGTVKKGYQMKVVKTVAVKILKNEANDPALKDELLAEANVMQQLDNPIYIRVMIGICEAESWMLVMEAEGLPLNKYLQQR

HVKDKNIIELVHQVSMGMKYLEESNFMVHRDLAARNVLLVTQHYAKISDFGLSKALRADENYYKAQTHGKWPVKWYAPECINYYKFSKSDVWSFGVLMWEAFSYGQKPYRGMKGSE

VTAMLEKGERMGPAGCPREMYDLMLNLQWYDVENRPGFAAVELRLRNYYDVVN

序列详情

Identifier	Method	Resolution	Chain	Positions	Source
1A81	X-Ray	3.0 Å	A/C/E/G/I/K	9 - 262	PDB
1CSY	NMR	-	A	163 - 265	PDB
1CSZ	NMR	-	A	163 - 265	PDB
1XBA	X-Ray	2.00 Å	A	353 - 635	PDB
1XBB	X-Ray	1.57 Å	A	353 - 635	PDB
1XBC	X-Ray	2.00 Å	A	353 - 635	PDB
3BUW	X-Ray	1.450 Å	A/C	317 - 329	PDB
				349 - 635	PDB

External Links and Identifiers

Alliance of Genome Resources: [HGNC:11491](#)

CHEMBL: [CHEMBL2599](#)

Ensembl gene: [ENSG00000165025.15](#), [ENSG00000165025](#)

HGNC: [HGNC:11491](#)

NCBI Gene: [6850](#)

OMIM: [600085](#)

Uniprot reviewed: [P43405](#)

[View Less](#)

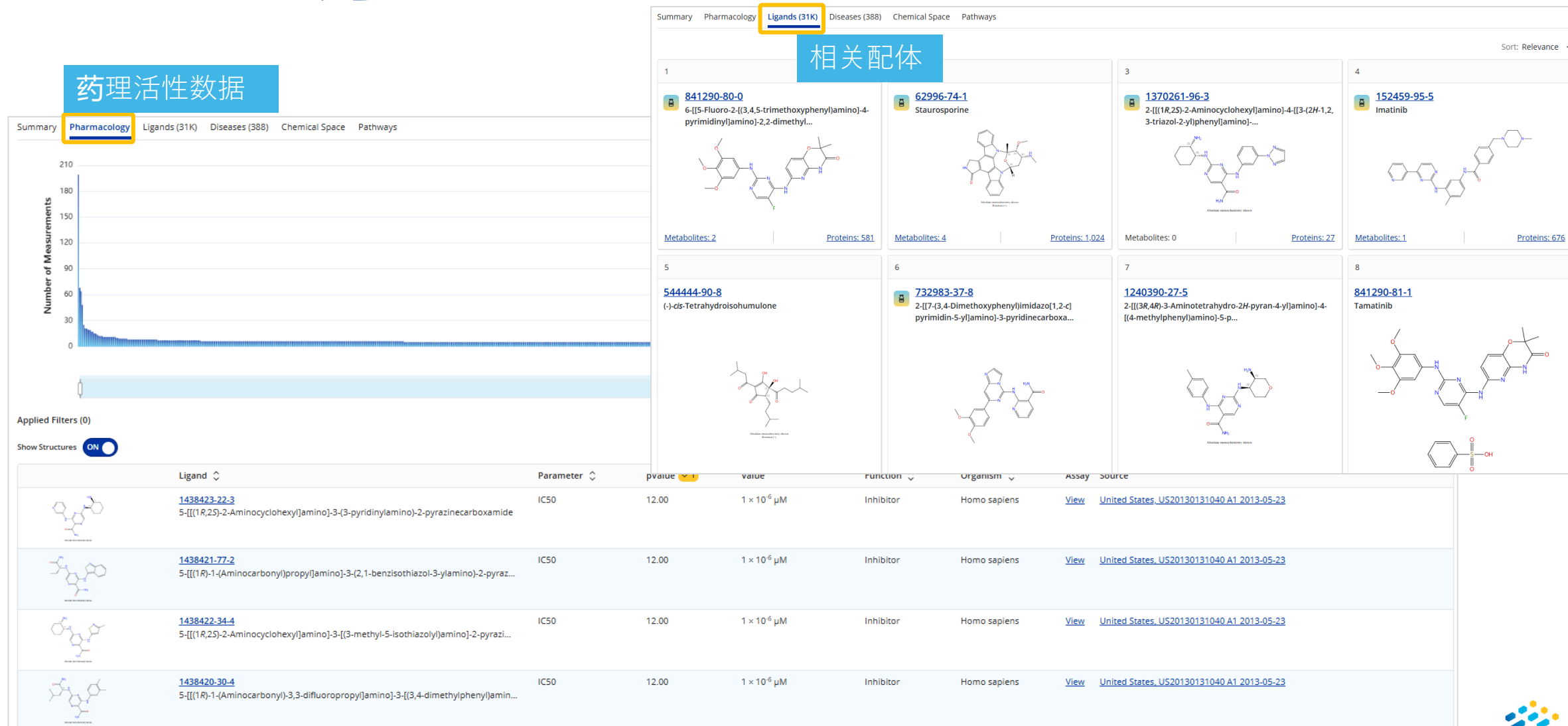
归一化的靶点名称与其他详情信息

Synonyms

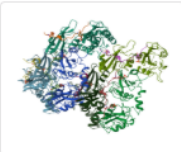
Spleen associated tyrosine kinase

Spleen tyrosine kinase

相关配体与药理活性数据



蛋白相关疾病信息



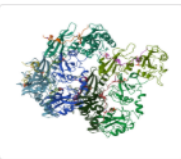
SYK
Tyrosine-protein kinase SYK

Summary Pharmacology Ligands (31K) **Diseases (388)** Chemical Space Pathways

Sort: Relevance ▾ [View all associated diseases](#)

Disease	疾病	Description	疾病描述	Biomarkers	生物标志物
1	Cancer	A disease of cellular proliferation that is malignant and primary, characterized by uncontrolled cellular proliferation, local cell invasion and metastasis.		BRCA1 DNA repair associated, Neurotrophin 4, Autophagy related 16 like 1, Major histocompatibility complex, class II, DP beta 1, KRAS proto-oncogene, GTPase, View All	7,479 1M
2	Alzheimer's disease	A tauopathy that is characterized by memory lapses, confusion, emotional instability and progressive loss of mental ability and results in progressive memory loss, impaired thinking, disorientation, and changes in personality and mood starting and leads in advanced cases to a profound decline in cognitive and physical functioning and is marked histologically by the degeneration of brain neurons especially in the cerebral cortex and by the presence of neurofibrillary tangles and plaques containing beta-amyloid.		Apolipoprotein E, Fibrinogen alpha chain, Islet amyloid polypeptide, APP (rs199862130) polymorphism, Synuclein alpha, View All	4,974 722K
3	Rheumatoid arthritis	An arthritis that is an autoimmune disease which attacks healthy cells and tissue located in joint.		TIMP metalloproteinase inhibitor 1, Solute carrier family 22 member 4, Tumor necrosis factor, Matrix metalloproteinase 1, Protein kinase C theta, View All	3,847 576K
4	Asthma	A bronchial disease that is characterized by chronic inflammation and narrowing of the airways, which is caused by a combination of environmental and genetic factors. The disease has symptom recurring periods of wheezing (a whistling sound while breathing), has symptom chest tightness, has symptom shortness of breath, has symptom mucus production and has symptom coughing.		Membrane spanning 4-domains A2, Transient receptor potential cation channel subfamily A member 1, Adrenomedullin, Fc epsilon receptor 1a, CDKN2B-AS1 (rs7859362) polymorphism, View All	3,333 516K
5	Diabetes mellitus	A glucose metabolism disease that is characterized by chronic hyperglycaemia with disturbances of carbohydrate, fat and protein metabolism resulting from defects in insulin secretion, insulin action, or both.		MTHFR (rs1801133) polymorphism, Cytokine inducible SH2 containing protein, Cystatin C, Insulin, Mechanistic target of rapamycin kinase, View All	3,871 401K

蛋白的生物通路信息



SYK
Tyrosine-protein kinase SYK

Summary Pharmacology Ligands (31K) Diseases (388) Chemical Space **Pathways**

Pathway 通路	Reaction 作用详情	Source 文献来源
alpha IIb beta3 pathway	Fibrinogen:(alpha IIb beta3)2:(Src)2 + 2 CIB:Ca + 2 talin <=> Fibrinogen:(alpha IIb beta3)2:(Src)2:(CIB)2:(Ca)2:(talin)2	Proceedings of the National Academy of Sciences of the United States of America (2003), 100(23), 13298-13302 Journal of Biological Chemistry (1997), 272(8), 4651-4654
	Rac1:GDP + GTP --VAV1{pY}:SLP-76{p}:Nck-1--> Rac1:GTP + GDP	EMBO Journal (1998), 17(22), 6608-6621 Journal of Biological Chemistry (2001), 276(8), 5916-5923
	alpha IIb beta3 + Csk + Src <=> alpha IIb beta3:Csk:Src	Journal of Cell Biology (2002), 157(2), 265-275
	Fibrinogen:(alpha IIb beta3)2:(Src{pY419})2:(CIB)2:(Ca)2:(talin)2:(Syk{pY})2 + 2 NDP	Biology (2002), 157(2), 265-275
	Fibrinogen + 2 alpha IIb beta3:Csk:Src{pY529}	Biology (2002), 157(2), 265-275
	SLP-76 + NTP --Fibrinogen:(alpha IIb beta3)2:	Journal of Biological Chemistry (2001), 276(8), 5916-5923 Journal of Biological Chemistry (1998), 273(48), 31890-31900
	vasp + SLAP-130{p} + SLP-76{p} <=> vasp:SLP-76{p}	Journal of Biological Chemistry (1996), 271(42), 25746-25749 Journal of Biological Chemistry (1995), 270(49), 29071-4 Journal of Biological Chemistry (2001), 276(8), 5916-5923
	Fibrinogen:(alpha IIb beta3)2:(Src{pY529})2 --	
	VAV1{pY}:SLP-76{p}:Nck-1 + PAK1 + Rac1:GTP	

Coordinate interactions of Csk, Src, and Syk kinases with alphaIIb beta3 initiate integrin signaling to the cytoskeleton

By: Oberfell, Achim; Eto, Koji; Mocsai, Attila; Buensuceso, Charito; Moores, Sheri L.; Brugge, Joan S.; Lowell, Clifford A.; Shattil, Sanford J.

DOI: 10.1083/jcb.200112113

Integrins regulate cell adhesion and motility through tyrosine kinases, but in contrast to the behavior of Src and Csk, Syk was associated with alphaIIb beta3 only after fibrinogen binding. Platelets multiply deficient in Src, Hck, Fgr, and Lyn, or normal platelets treated with Src kinase inhibitors failed to spread on fibrinogen. Inhibition of Src kinases blocked Syk activation and inhibited phosphorylation of Syk substrates (Vav1, Vav3, SLP-76) implicated in cytoskeletal regulation. Syk-deficient platelets exhibited Src activation upon adhesion to fibrinogen, but no spreading or phosphorylation of Vav1, Vav3, and SLP-76. These studies establish that platelet spreading on fibrinogen requires sequential activation of Src and Syk in proximity to alphaIIb beta3, thus providing a paradigm for initiation of integrin signaling to the actin cytoskeleton.

Keywords: Csk Src Syk kinase integrin signaling cytoskeleton platelet adhesion

[View Source](#) [Full Text](#)

Publication Information • Journal

Source	Database Information	Company/Organization	Publisher	Language
Journal of Cell Biology Volume: 157 Issue: 2 Pages: 265-275 Journal: Article: Research Support, Non-U.S. Gov't; Research Support, U.S. Gov't; P.H.S. 2002 DOI: 10.1083/jcb.200112113	AN: 2002:296764 CAN: 137:106866 PubMed ID: 11940607 Cajupus and MEDLINE	Division of Vascular Biology, Department of Cell Biology The Scripps Research Institute La Jolla, California 92037 United States	Rockefeller University Press	English

一键链接到SciFinder文献详情页

通过疾病名称、靶点或配体，检索相关疾病信息

CAS

BioFinder

Diseases

APP

← Return to all Filters

Biomarker

Enter a Biomarker...

Search

0 Selected

☐ Insulin

☐ Hemoglobin subunit alpha 2

☐ Hemoglobin subunit alpha 1

☐ Hemoglobin subunit beta

☐ Epidermal growth factor receptor

☐ C-reactive protein

☐ Erb-b2 receptor tyrosine kinase

☐ Microtubule associated protein tau

☐ Estrogen receptor

☐ Tumor necrosis factor

☐ Interleukin 6

☐ Apolipoprotein E

☐ Kallikrein related peptidase 3

☐ Synuclein alpha

☐ KRAS proto-oncogene, GTPase

☐ Adiponectin, C1Q and collagen domain containing

☐ BRCA1 DNA repair associated

☐ AKT serine/threonine kinase 1

☐ Androgen receptor

☐ Leptin

☐ Vascular endothelial growth factor A

☐ Glucagon

☐ Angiotensin I converting enzyme

☐ Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit alpha

☐ Amyloid beta precursor protein

通过生物标志物进行筛选

Diseases search for APP

Diseases

172 Results

Sort: Relevance

疾病名称	疾病简介	生物标志物	相关靶点与配体
1 Cancer	A disease of cellular proliferation that is malignant and primary, characterized by uncontrolled cellular proliferation, local cell invasion and metastasis.	BRCA1 DNA repair associated, Neurotrophin 4, Autophagy related 16 like 1, Major histocompatibility complex, class II, DP beta 1, KRAS proto-oncogene, GTPase, View All	7,479 1M
2 Alzheimer's disease	A tauopathy that is characterized by memory lapses, confusion, emotional instability and progressive loss of mental ability and results in progressive memory loss, impaired thinking, disorientation, and changes in personality and mood starting and leads in advanced cases to a profound decline in cognitive and physical functioning and is marked histologically by the degeneration of brain neurons especially in the cerebral cortex and by the presence of neurofibrillary tangles and plaques containing beta-amyloid.	Apolipoprotein E, Fibrinogen alpha chain, Islet amyloid polypeptide, APP (rs199862130) polymorphism, Synuclein alpha, View All	4,974 722K
3 Rheumatoid arthritis	An arthritis that is an autoimmune disease which attacks healthy cells and tissue located in joint.	TIMP metalloproteinase inhibitor 1, Solute carrier family 22 member 4, Tumor necrosis factor, Matrix metalloproteinase 1, Protein kinase C theta, View All	3,847 576K
4 Asthma	A bronchial disease that is characterized by chronic inflammation and narrowing of the airways, which is caused by a combination of environmental and genetic factors. The disease has symptom recurring periods of wheezing (a whistling sound while breathing), has symptom chest tightness, has symptom shortness of breath, has symptom mucus production and has symptom coughing.	Membrane spanning 4-domains A2, Transient receptor potential cation channel subfamily A member 1, Adrenomedullin, Fc epsilon receptor 1a, CDKN2B-AS1 (rs7859362) polymorphism, View All	3,333 516K
5 Diabetes mellitus	A glucose metabolism disease that is characterized by chronic hyperglycaemia with disturbances of carbohydrate, fat and protein metabolism resulting from defects in insulin secretion, insulin action, or both.	MTHFR (rs1801133) polymorphism, Cytokine inducible SH2 containing protein, Cystatin C, Insulin, Mechanistic target of rapamycin kinase, View All	3,871 401K
6 Bacterial infectious disease	A disease by infectious agent that results in infection, has material basis in Bacteria.	Tumor necrosis factor, Activation induced cytidine deaminase, Serum amyloid A1, Transforming growth factor beta 1, C-C motif chemokine ligand 17, View All	2,645 202K
7 Parkinson's disease	A synucleinopathy that has material basis in degeneration of the central nervous system that often impairs motor skills, speech, and other functions.	Synuclein alpha, Leucine rich repeat kinase 2, Ubiquitin C-terminal hydrolase L1, Glucosylceramidase beta 1, Mechanistic target of rapamycin kinase, View All	4,497 423K
8 Psoriasis	A skin disease that is characterized by patches of thick red skin and silvery scales.	Interleukin 1 beta, Insulin, C-C motif chemokine ligand 5, Acyl-CoA thioesterase 12, ADAM metalloproteinase domain 10, View All	2,937 430K

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疾病详情页与相关药物信息

Alzheimer's disease

相关生物标志物、药理活性数据、配体与靶点

Summary

Biomarkers

Pharmacology

Ligands (705K)

Proteins (4,937)

A tauopathy that is characterized by memory lapses, confusion, emotional instability and progressive loss of mental ability and results in progressive memory loss, impaired thinking, disorientation, and changes in personality and mood starting and leads in advanced cases to a profound decline in cognitive and physical functioning and is marked histologically by the degeneration of brain neurons especially in the cerebral cortex and by the presence of neurofibrillary tangles and plaques containing beta-amyloid.

Synonyms

Aging-related Alzheimer's disease
Alzheimer disease
Alzheimer's
Alzheimer's senile dementia
Alzheimer's type dementia
Alzheimers dementia
Early onset Alzheimer's disease
Intermediate-stage Alzheimer's disease
Late onset Alzheimer's disease

[View Less](#)

External Links and Identifiers

GARD: [10254](#)
KEGG: [05010](#)
MESH: [D000544](#)
NCI: [C2866](#)

疾病简介

归一化的疾病 同义词列表

AI Drug Intelligence Summarization

AI总结药物情报信息

Here is a summary of the state of drugs used to treat Alzheimer's disease:

CAS BioFinder shows 327 drug entries targeting Alzheimer's disease, predominantly consisting of small molecule compounds. The drugs exhibit diverse mechanisms of action, targeting various biological pathways including cholinergic signaling (acetylcholinesterase inhibitors, neuronal acetylcholine receptor agonists), kinase pathways (tyrosine kinase inhibitors targeting c-Kit, PDGFR, and Lyn), neurotransmitter systems (sigma opioid receptor agonists, serotonin 5-HT4 receptor agonists), and cellular signaling (glycogen synthase kinase-3 beta inhibitors, voltage-gated calcium channel blockers). The therapeutic approaches include both primary treatments aimed at disease modification and palliative treatments for symptom management. Development phases range from early Phase I studies to Phase III trials, with some compounds having achieved approved status. Target functions encompass inhibitors, agonists, partial agonists, and blockers, reflecting the multifaceted approach to addressing the complex pathophysiology of Alzheimer's disease through modulation of neuroinflammation, neurotransmission, and neuroprotective pathways.

This is an AI-generated summary of the drug intelligence information, and may be incomplete or include some inaccuracies. Please consult the records in the table for the source empirical data.

CAS BioFinder AI is always improving. [suggest improvements](#), or [learn more](#).

DRUGS

药物情报信息列表

Ligand	Modality	Highest Phase	Source
98185-20-7 Raclopride tartrate	Diagnostic	Approved	-
1098-97-1 Pyritinol	Primary	Approved	Dementia (Base, Switzerland) (0, 5(2), 88-98)
23173-12-8 <i>rel</i> -(4a <i>R</i> ,6 <i>S</i> ,8a <i>R</i>)-4a,5,9,10,11,12-Hexahydro-3-methoxy-11-methyl-6 <i>H</i> -benzofuro[3a,3...	Palliative	Approved	Source
86332-23-2 1,2,3-Propanetriol, 2-(dihydrogen phosphate), monopotassium salt	Palliative	Approved	Source
120011-70-3 Donepezil hydrochloride	Palliative	Approved	Source

疾病与生物标志物

AI Table Summarization

There are 24 top biomarkers for Alzheimer's disease:

Select a biomarker to see more details.

[Microtubule associated protein tau](#), [Amyloid beta precursor protein](#), [Apolipoprotein E](#), [Tumor necrosis factor](#), [Insulin](#), [Brain derived neurotrophic factor](#), [Glycogen synthase kinase 3 beta](#), [Insulin like growth factor 1](#), [Triggering receptor expressed on myeloid cells 2](#), [Presenilin 1](#), [Acetylcholinesterase \(Yt blood group\)](#), [ATP binding cassette subfamily A member 7](#), [Butyrylcholinesterase](#), [Beta-secretase 1](#), [Sortilin related receptor 1](#), [Angiotensin I converting enzyme](#), [Granulin precursor](#), [Synuclein alpha](#), [Glutamate ionotropic receptor NMDA type subunit 2B](#), [Clusterin](#), [Interleukin 1 beta](#), [Presenilin 2](#), [Advanced glycosylation end-product specific receptor](#), [Translocase of outer mitochondrial membrane 40](#)

AI总结

Alzheimer's disease

Summary **Biomarkers** Pharmacology Ligands (722K) Proteins (4,974)

生物标志物

参数

实验说明

有机体

文献来源

Show Filters

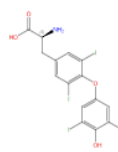
Summarize



Biomarker	Gene	Category	Parameter	Measurement	Organism	Assay	Source
(-)-Thyroxine	-	Diagnostic	Biomarker level	Mean free Thyroxine (FT4) level was observed in 40 patients with alzheimer's disease with blunted TSH response which is significantly (P<0.01) more severely demented when compared to patients with non blunted TSH response.	Human	View	Biological psychiatry (0, 30(6), 567-76

(-)-Thyroxine Detail

Biomarker
[51-48-9](#)



L-Tyrosine, O-(4-hydroxy-3,5-diiodophenyl)-3,5-diiodo-

实验详情

Category	Diagnostic
Parameter	Biomarker level
Measurement	Mean free Thyroxine (FT4) level was observed in 40 patients with alzheimer's disease with blunted TSH response which is significantly (P<0.01) more severely demented when compared to patients with non blunted TSH response, Mean free Thyroxine(FT4) level was observed in 40 patients with alzheimer's disease having blunted TSH response which was significantly (P<0.03) higher when compared to patients with non blunted TSH response, High, Mean Thyroxine (T4) level was observed in 40 alzheimer's disease patients which is significantly (P<0.05) lower when compared to 17 elderly patients with major depression, Low
Organism	Human
Source	Biological psychiatry (0, 30(6), 567-76

提纲

- CAS BioFinder 简介与检索界面介绍 (Introduction and Interface)
- 配体检索与配体详情信息 (Ligands and Details Overview)
- 骨架检索与构效关系分析 (Scaffolds and SAR Analysis)
- 蛋白/通路/靶点、疾病与生物标志物 (Proteins & Pathways; Diseases & Biomarkers)
- 生物活性预测 (Predictive Analytics)

Predictive Analytics：通过算法预测配体对不同靶点的生物活性数据

The image illustrates the workflow for creating a predictive analytics set in the CAS software. It starts with the main dashboard where the 'Predictive Analytics' section is highlighted. An arrow points to the 'Create New Set' button in the 'Predictive Sets (24)' tab. This leads to the 'Create Predictive Analytics Set' dialog box. In this dialog, the 'Name your set' field is populated with 'Predictive_Set_09_09_2025_0952' and the 'Select Color' dropdown is set to 'Light Blue'. The 'Select Panel' dropdown is open, showing a list of predefined panels including 'CAS Full Pharmacology (Default)', 'CAS Broad Safety Screen', 'CAS Medium Safety Screen', 'CAS Narrow Safety Screen', 'CAS Alzheimer's Disease Screen', 'CAS Breast Cancer Screen', 'CAS Colon Cancer Screen', and 'CAS Depressive Disorder Screen'. A blue callout box points to this dropdown with the text '选择不同的预测面板'. Below the dropdown, there is a text input area for uploading a predefined set, with a blue callout box pointing to it that says '上传.sdf文件'. At the bottom of the dialog are 'Create' and 'Cancel' buttons. A yellow arrow points from the 'Create' button to a context menu that appears when clicking on a set in the 'Predictive Sets' list. This menu contains the following options: 'Rerun analysis for set', 'Add ligands from file', 'Edit set', and 'Delete set'.

Create Predictive Analytics Set

Name your set: Predictive_Set_09_09_2025_0952

Select Color: Light Blue

Select Panel: CAS Full Pharmacology (Default)

Upload a predefined set (Optional):

- CAS Full Pharmacology (Default)
- CAS Broad Safety Screen
- CAS Medium Safety Screen
- CAS Narrow Safety Screen
- CAS Alzheimer's Disease Screen
- CAS Breast Cancer Screen
- CAS Colon Cancer Screen
- CAS Depressive Disorder Screen

Select a file (.sdf) or drag and drop here.

Create Cancel

Predictive Test XXX

CAS Full Pharmacology (Default) - Complete

Ligands: 1	Neighbors: 191 Metabolites: 7	Targets: 111
------------	----------------------------------	--------------

Updated on 29 August 2025

Rerun analysis for set
Add ligands from file
Edit set
Delete set

可从检索结果集中添加配体结构

Filters

Chemical Filters

OFF

Rule of 5 Filter Preset
This will automatically be applied.

pValue

Modality

Druglikeness

ADME

Commercial Availability

Approval Status

Approval Authority

Biological Filters

Target

Target Type

Disease

Organism

Parameter

Function

Experiment Type

Ligands search for drawn structure

Ligands

ScaffoldsPharmacology

25 of 9,190 Selected

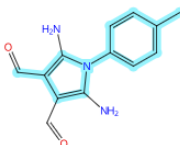
Sort: Relevance

Predictive Analytics

1

1961259-82-4

2,5-Diamino-1-(4-methylphenyl)-1H-pyrrole-3,4-dicarboxaldehyde

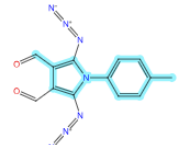


Metabolites: 2 | Proteins: 0

2

1961259-76-6

2,5-Diazo-1-(4-methylphenyl)-1H-pyrrole-3,4-dicarboxaldehyde

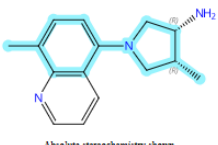


Metabolites: 2 | Proteins: 0

3

2270167-74-1

(3R,4R)-4-Methyl-1-(8-methyl-5-quinolinyl)-3-pyrrolidinamine

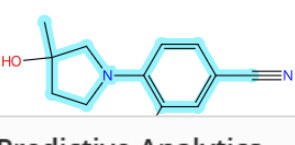


Metabolites: 4 | Proteins: 2

4

2002854-95-5

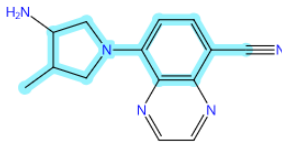
4-(3-Hydroxy-3-methyl-1-pyrrolidinyl)-3-methylbenzonitrile



5

2270167-41-2

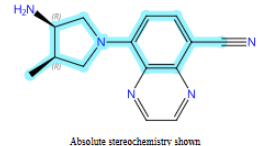
8-(3-Amino-4-methyl-1-pyrrolidinyl)-5-quinoxalinecarbonitrile



6

2270167-40-1

8-[(3R,4R)-3-Amino-4-methyl-1-pyrrolidinyl]-5-quinoxalinecarbonitrile

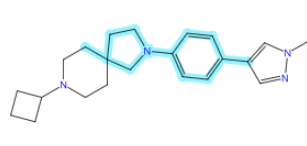


Absolute stereochemistry shown

7

1067895-50-4

8-Cyclobutyl-2-[4-(1-methyl-1H-pyrazol-4-yl)phenyl]-2,8-diazaspiro[4.5]decane



Predictive Analytics

Create New Set

Add to Existing Set

Name your set

Predictive_Set_09_09_2025_1002

Select Color

Light Blue

Select Panel

CAS Breast Cancer Screen

25 selected ligands will be added to this set

Create

Cancel

43

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不同的蛋白靶点面板说明

History (407) Predictive Sets (25)

Create New Set Panels

Predictive Set CAS Breast Cancer Screen

Ligands: 25

Updated on 09 September

Search panels by name...

Panel Name	Description	Targets
CAS Full Pharmacology (Default)	The full panel of protein target models available through CAS to highlight potential safety concerns and treatment options	All
CAS Broad Safety Screen	A diverse panel of protein targets to widely test the safety of your drug candidate	192
CAS Medium Safety Screen	Panel of protein targets likely to be implicated to adverse drug reactions (ADRs) based off of known structure activity relationships (SARs)	115
CAS Narrow Safety Screen	Panel of protein targets established as being involved in adverse drug reactions (ADRs). These targets are essential for early safety screening of drugs	49
CAS Alzheimer's Disease Screen	Panel of protein targets potentially implicated in Alzheimer's Disease	81
CAS Breast Cancer Screen	Panel of protein targets potentially implicated in breast cancer and neoplasms	70
CAS Colon Cancer Screen	Panel of protein targets potentially implicated in colon cancer and neoplasms	92
CAS Depressive Disorder Screen	Panel of protein targets potentially implicated in depressive disorder and major depressive disorder	51
CAS Diabetes Screen	Panel of protein targets potentially implicated in diabetes	78
CAS Inflammation Screen	Panel of protein targets potentially implicated in inflammation	33
CAS Liver Cancer Screen	Panel of protein targets potentially implicated in liver cancer and neoplasms	73
CAS Lung Cancer Screen	Panel of protein targets potentially implicated in lung cancer and neoplasms	66
CAS Parkinson's Disease Screen	Panel of protein targets potentially implicated in Parkinson's disease	46
CAS Prostate Cancer Screen	Panel of protein targets potentially implicated in prostate cancer and neoplasms	70

点击查看详细靶点名称列表

自定义靶点面板

Panels

+ Create New Panel

Search panels by name...

Panel Name	Description
CAS Full Pharmacology (Default)	The full panel of protein target models available through CAS to highlight potentia
Predictive_Panel_Test	

Panel Name

Predictive_Panel_Test

Description (Optional)

Cancel

Create Panel

Targets to Include in Panel

Target

Organism

Uniprot ID

☒	Prostaglandin F2-alpha receptor	Felis catus	6L9K4
☒	Gag-pol polyprotein	Escherichia coli	A0A0A0F4Y0
☒	Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform	Rattus norvegicus	A0A0G2K344
☒	Dihydroorotate dehydrogenase (quinone)	Plasmodium falciparum Dd2	A0A0L7M6L3
☒	Bifunctional dihydrofolate reductase-thymidylate synthase	Cryptosporidium hominis	A0A054TER9
☐	Dihydrofolate reductase	Cryptosporidium hominis	A0A0W0CF37
☐	Beta-glucuronidase	Escherichia coli BL21(DE3)	A0A140N7P8
☐	Methionine aminopeptidase	Escherichia coli	A0A193LMB0
☐	Glucose-dependent insulinotropic receptor	Mesocricetus auratus	A0A1U8CD06
☐	Matrix protein 2	Influenza A virus (A/WSN/1933(H1N1))	A0A1Y0AWW2
☐	Delta-type opioid receptor	Cavia porcellus	A0A286XTF2
☐	Emopamil-binding protein-like	Cavia porcellus	A0A286XUI8
☐	5-hydroxytryptamine receptor 2C	Cavia porcellus	A0A286XYP5
☐	5-hydroxytryptamine receptor 1A	Cavia porcellus	A0A286Y074
☐	Thromboxane A2 receptor	Cavia porcellus	A0A286Y4I8

Selected Targets

Prostaglandin F2-alpha receptor (Felis catus)

Gag-pol polyprotein (Escherichia coli)

Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform (Rattus norvegicus)

Dihydroorotate dehydrogenase (quinone) (Plasmodium falciparum Dd2)

Bifunctional dihydrofolate reductase-thymidylate synthase (Cryptosporidium hominis)

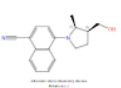
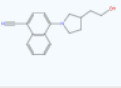
Can自定义面板名称

45

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生物活性预测结果

[Return to Predictive Analytics](#)
Predictive_Set_09_09_2025_1002
Ligands **Pharmacology**
Show Structures **ON**
Total ligands: 25
Neighbors: 78
Metabolites: 53
Targets: 21
Filters
pActivity
Confidence Score
Target
☐ Androgen receptor
☐ Progesterone receptor
☐ Tumor necrosis factor
☐ Glycogen synthase kinase-3 beta
☐ Estrogen receptor
[View All](#) [Apply](#)
Organism
[Return to top](#)

Ligand	Target	Organism	Known pAct	Predicted pAct	Confidence	Method
 664363-58-0	Androgen receptor	Homo sapiens	8.39	8.26	0.8	●●●●●
 664363-91-1	Progesterone receptor	Homo sapiens	-	8.02	0.39	●●●●●
 664363-58-0	Progesterone receptor	Homo sapiens	-	8.01	0.39	●●●●●
 664363-52-4	Progesterone receptor	Homo sapiens	-	7.95	0.39	●●●●●
 664363-02-4	Androgen receptor	Homo sapiens	-	7.94	0.79	●●●●●
 664363-02-4	Progesterone receptor	Homo sapiens	-	7.94	0.39	●●●●●

可直接链接到相关靶点详情页

从左到右涉及的方法有：
MLM, SAS, SEA, SIM, XPI使用左侧筛选功能可对这些数据进行细化分析：

- 活性值(pActivity)
- 置信度分数(Confidence score)
- 靶点(Target)
- 有机体(Organism)

助于探索特定范围内的pAct, 或有较高可信度的预测信息。

总结

配体检索 (Ligands)

- 基于**药物名称**、**CAS RN**、**结构**、**靶点**、**疾病**等，**获取配体信息**
- 通过**类药性**、**ADME**、**实验参数**、**药物功能**、**生物有机体**等，**进行筛选聚焦**
- **查看并评估**化合物的**药理学**、**ADME**、**毒理学**和**代谢物**信息及**可视化展示**

骨架检索 (Scaffolds)

- 基于**结构**或**靶点**等信息，**高效获取**相关**骨架结构**，并通过**官能团R-Groups**，**进行构效关系分析**
- 通过 **SAR** 以及**MMPA**，**优化目标骨架**或**先导化合物**的**效力**和**选择性**
- 探索**针对**关注**靶点**同一**结构骨架**中**活性最高**的**配体**，**获取相似骨架结构**与**拓展**

蛋白/通路/靶点与疾病检索(Proteins & Diseases)

- **高效获取**蛋白质**通路/靶点**与**疾病生物标志物**信息，探索**药物作用机制**和**适应症**

预测配体与不同靶点的生物活性(Predictive Analytics)

- **预测**特定**结构****针对**特定**靶点**的**药理活性**信息
- 关注配体的**脱靶效应**与**药物再利用**

相关资源 Learn More

<https://biofinder.cas.org/>

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and progress **are**
connections that
matter

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