

CAS BIOFINDER DISCOVERY PLATFORM™
快速使用指南 (QUICK GUIDE)



大綱

- CAS BioFinder簡介與界面介紹
- 配體檢索與配體詳情信息（配體與細節概述）
- 骨架檢索與構效關係分析（支架與搜救分析）
- 蛋白/通路/靶點、疾病與生物標誌物（Proteins and Pathways;疾病與生物標記）
- 生物活性預測（Predictive Analytics）

科學資訊管理對新葯研發至關重要

低增長時代的特點對創新的要求極大提升，而在當今的創新環境下，數據管理任務艱巨

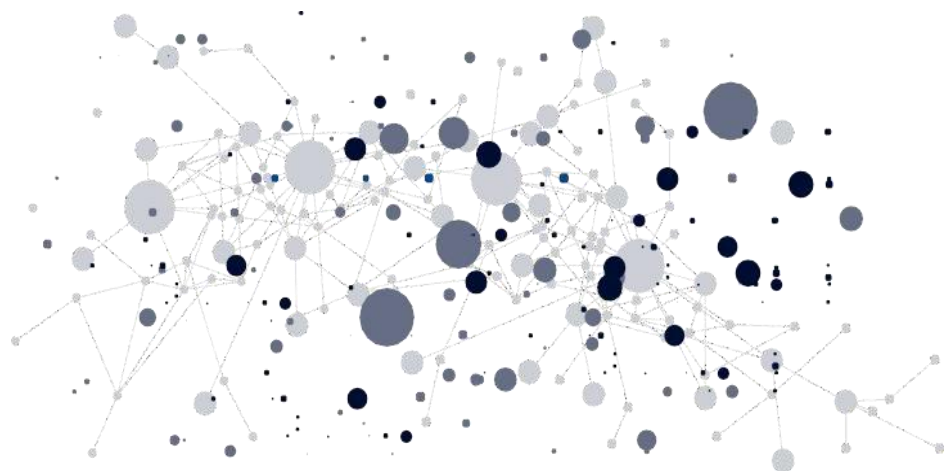
- 信息鴻溝會導致創新管線薄弱、研發效率低下，以及意外的知識產權風險
- 由於數據量和數據類型日益複雜，藥物發現流程中，整合和分析關鍵的研發數據資訊，對於迅速做出關鍵決策至關重要。
- 持續的數據管理有助於開發差異化的成果，支撐創新藥物的發現，確保藥物研發成功進入審批階段，並可避免後續智慧財產權問題。

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

生命科學領域研究離不開重要的數據資訊基礎， 但為什麼卻難以加以利用？

缺乏關聯性

生命科學研究和數據分散在各個資料庫、
期刊和專利等眾多互不關聯的資源之中



未一致化

不同資源對相同資訊的描述各不相同，
因此很難對數據進行分析和比較



數據問題導致延緩創新進程，增加財務風險

遺漏見解



這些見解能夠為研究人員制定研發戰略提供指導

僅在美國，每年就有5,000到6,000起專利侵權和專利無效的訴訟，法院判定的賠償金額接近 50 億美元¹。

耗費時間



生命科學數據量每 14 年翻一番²

數據科學家將 50%-80% 的時間都花費在收集和整理用於分析模型的數據資訊的瑣碎的工作中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 加速早期藥物研發



CAS BioFinder 檢索介面

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



Draw



CAS Newton

Chat with CAS Newton to answer your drug discovery questions.



Predictive Analytics

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



Search Sequences **BETA**

Query BLAST algorithms for nucleotide and protein based sequences.

結構繪製面板

活性預測分析 (基於演算法, 預測某一個或多個結構與不同靶點的生物活性數據)

Recent Search History

[View Search History](#)

7 May 2026

近期檢索歷史

CAS Newton

Research

10:14 AM

雙特異抗體中靶點是pd1-vegfr的藥物

View Results



Search Complete

Edit search
Delete search

大綱

- CAS BioFinder簡介與檢界面介紹（介紹與介面）
- 配體檢索與配體詳情信息（配體與細節概述）
- 骨架檢索與構效關係分析（支架與搜救分析）
- 蛋白/通路/靶點、疾病與生物標誌物（Proteins and Pathways; 疾病與生物標記）
- 生物活性預測（Predictive Analytics）

基於靶點、疾病、藥物名稱以及結構，檢索資訊

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

自動提示敘詞表

CAS BioFinder

Ligands BTK

Filters

Chemical Filters

Rule of 5 Filter Preset OFF 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

藥物情報信息標識

1 936563-96-1 Ibrutinib

2 1420477-60-6 4-[8-Amino-3-[(2S)-1-(1-oxo-2-butyn-1-yl)-2-pyrrolidinyl]imidazo[1,5- σ]pyrazin-1...

3 1691249-45-2 (7S)-4,5,6,7-Tetrahydro-7-[1-(1-oxo-2-propen-1-yl)-4-piperidinyl]-2-(4-phenoxyph...

4

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

Metabolites: 3 | Proteins: 687

Metabolites: 0 | Proteins: 203

Metabolites: 0 | Proteins: 36

Metabolites: 7 | Proteins: 215

5 2095280-64-9 N-[3-[1,6-Dihydro-1-methyl-5-[[4-(4-

6 2095280-65-0 N-[3-[1,6-Dihydro-1-methyl-5-[[4-(4-

7 1803358-13-5 N-[2-Methyl-5-[2-oxo-9-(1H-pyrazol-1-

8 910232-84-7 N-[3-[4,5-Dihydro-4-methyl-6-[[4-(4-

篩選具有類似先導化合物特性的小分子配體

一鍵應用Rule of 5

Chemical Filters

Rule of 5 Filter Preset
This will automatically be applied.

ADME

Partition Coefficient (logP)
-1.17 to 7.18

Solubility (logS)
-8.94 to 0.58

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

Permeability Glycoprotein (Pgp)
0 to 1

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

Plasma Protein Binding (PPB)
16 to 100

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

Modality

Druglikeness

Hydrogen Bond Acceptors
2 to 13

Hydrogen Bond Donors
0 to 7

Freely Rotatable Bonds
0 to 13

Molecular Weight (g/mol)
260 to 587

Molar Refractivity (m³/mol)
58 to 152

Number of Atoms
11 to 36

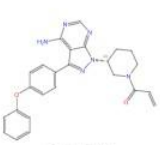
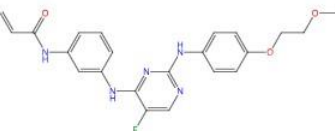


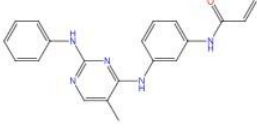
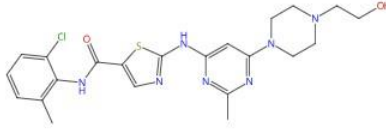
[Reset Filter](#) [Apply](#)

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

<p>1</p> <p>936563-96-1 Ibrutinib</p>  <p>Metabolites: 3 Proteins: 687</p>	<p>2</p> <p>1202757-89-8 CC 292</p>  <p>Metabolites: 7 Proteins: 215</p>	<p>3</p> <p>1803358-13-5 N-[2-Methyl-5-[2-oxo-9-(1H-pyrazol-1-yl)benzo[h]-1,6-naphthyridin-1(2H)-yl]phenyl]...</p>  <p>Metabolites: 7 Proteins: 16</p>
<p>5</p> <p>1803358-31-7 N-[2-Methyl-5-[2-oxo-9-(1H-pyrazol-1-yl)benzo[h]-1,6-naphthyridin-1(2H)-yl]phenyl]...</p>  <p>Metabolites: 8 Proteins: 15</p>	<p>6</p> <p>1202755-92-7 N-[3-[[5-Methyl-2-(phenylamino)-4-pyrimidinyl]amino]phenyl]-2-propenamide</p>  <p>Metabolites: 12 Proteins: 12</p>	<p>7</p> <p>302962-49-8 Dasatinib</p>  <p>Metabolites: 4 Proteins: 733</p>
<p>9</p> <p>1415823-49-2 1-[4-[[[6-Amino-5-(4-phenoxyphenyl)-4-pyrimidinyl]amino]methyl]-</p>	<p>10</p> <p>1202755-89-2 (2E)-4-(Dimethylamino)-N-[3-[[5-fluoro-4-[[3-methylphenyl]amino]-</p>	<p>11</p> <p>1202757-97-8 1-[[[3R]-3-[[5-Fluoro-2-[[3-methoxyphenyl]amino]-4-pyrimidinyl]oxy]</p>

- 氫鍵受體 <10
- 氫鍵供體 <5
- 自由旋轉鍵 <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

配體檢索結果的縱覽與聚焦

The screenshot displays the CAS BioFinder interface for a search on BTK. The main search results are organized into a grid of cards, each showing a chemical structure, a CAS ID, and a name. The interface includes several filter panels on the left and right.

Left Panel: Disease

- Search box: Enter a Disease... Search
- Annotations: 可通過檢索進行篩選聚焦
- Annotations: 靶点 (Target), 疾病 (Disease)

Top Left Panel: Filters

- Chemical Filters: Rule of 5 Filter Preset (OFF)
- Modality (highlighted)
- Druglikeness
- ADME
- Commercial Availability
- Approval Status (highlighted)
- Approval Authority
- Biological Filters: Target, Target Type, Disease, Organism, Parameter, Function, Experiment Type
- Annotations: 有機參數功能 (Organic Parameter Function), 實驗類型 (Experiment Type)

Top Right Panel: Modality

- Annotations: 小分子 (Small Molecule), 蛋白/肽类 (Protein/Peptide), 配合物 (Coordination Compound), 抗体 (Antibody), ADC, 聚合物 (Polymer)

Bottom Right Panel: Approval Status

- Annotations: 小分子 (Small Molecule), 蛋白/肽类 (Protein/Peptide), 配合物 (Coordination Compound), 抗体 (Antibody), ADC, 聚合物 (Polymer)

Search Results Grid

- 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

縱覽配體檢索結果集相關骨架結構與藥理學數據

查看配體檢索結果
關聯的骨架結構

Ligands search for BTK

Ligands **Scaffolds** Pharmacology

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

10,870 Results

1

Ligands: 1 | Proteins: 1

2

Ligands: 1 | Proteins: 1

5

Ligands: 1 | Proteins: 1

6

Ligands: 1 | Proteins: 1

7

Ligands: 1 | Proteins: 1

8

Ligands: 1 | Proteins: 2

Ligands search for BTK

Ligands Scaffolds **Pharmacology**

Number of Measurements

60K
50K
40K
30K
20K
10K
0

數據可視化:

- 柱狀/折線圖：每條柱形/折線節點
- 代表針對不同靶點的測量實驗數量調節圖下方的橫條，可放大圖表的特定區域

Tyrosine-protein kinase BTK 56K Measurements

Number of Measurements

60K
50K
40K
30K
20K
10K
0

Show Structures **ON** 顯示配體結構

Ligand	Target	Gene	Parameter	pValue	Value	Function	Assay	Source
 868540-17-4 Carfilizomib	MV4-11 cell (Cell line)	-	IC50	17.06	8.67×10^{-12} μ M	Inhibitor	View	ChemMedChem(2019)_14(23)_2005-2022
 868540-17-4 Carfilizomib	MV4-11 cell (Cell line)	-	IC50	16.88	1.33×10^{-11} μ M	Inhibitor	View	ChemMedChem(2019)_14(23)_2005-2022
 868540-17-4 Carfilizomib	MV4-11 cell (Cell line)	-	IC50	16.63	2.34×10^{-11} μ M	Inhibitor	View	ChemMedChem(2019)_14(23)_2005-2022
 868540-17-4 Carfilizomib	MV4-11 cell (Cell line)	-	IC50	16.50	3.15×10^{-11} μ M	Inhibitor	View	ChemMedChem(2019)_14(23)_2005-2022
 868540-17-4 Carfilizomib	THP-1 cell (Cell line)	-	IC50	16.40	4.01×10^{-11} μ M	Inhibitor	View	ChemMedChem(2019)_14(23)_2005-2022

可下載表格中的
的詳細數據

點擊View，可查看原
文中的Assay的細節

探索配體的詳細資訊

Doxorubicin

CAS Registry Number: 23214-92-8

View Associated Scaffold | View in CAS SciFinder

112K | 1,642 | Retrosynthesis | Predictive Analytics

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

配體相關信息標籤頁

藥物情報資訊

配體屬性資訊

H bond acceptors*	H bond donors*	Molecular weight (g/mol)	Molar refractivity (m³/mol)	Number of atoms	Freely rotatable bonds*	logP*	logS	logBB	Polar surface area (Å²)*	Plasma protein binding	Permeability glycoprotein
12	7	543.52	133.94	39	5	0.918	-3.27	-1.96	206.07	67.32	1

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

配體結構資訊與其他名稱

Canonical SMILES
O=C1C=C2C=CC=C(C(OC)C2(=O)C=C3C(=O)C13)CC(O)(C(=O)CO)C4C5OC(C(C)O)C(N)C5

Isomeric SMILES
OC=C1C2=C([C@@H]1O)[C@@H]3C[C@H](N)[C@@H]4O[C@H](C3)C[C@@]4(C(CO)=O)(O)C2(C)O=C4C1C(=O)C=5C(C4=O)=C(O)C=C5

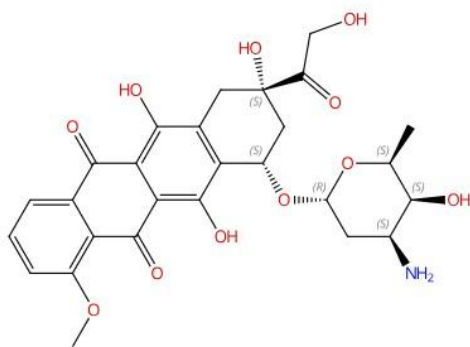
InChI
InChI=1S/C27H29NO11/c1-10-22(31)3(28)6-17(38-10)39-15-8-27(36,16(30)9-29)7-12-19(15)26(35)21-20(24(12)33)23(32)11-4-3-5-14(37-2)18(11)25(21)34/h3-5,10,13,15,17,22,29,31,33,35-36H,6-9,28H2,1-2H3/t10-,13-,15-,17-,22+,27-/m0/s1

InChI Key
A0JJSUZBOXZQNB-TZSSRYMLSA-N

22 other names for this Ligand

- (7S,9S)-7-([(2R,4S,5S,6S)-4-Amino-5-hydroxy-6-methylxan-2-yl]oxy)-6,9,11-trihydroxy-9-(2-hydroxyacetyl)-4-methoxy-8,10-dihydro-7H-tetracene-5,12-dione
- (8S,10S)-10-[(3-Amino-2,3,6-trideoxy-α-L-lyxo-hexopyranosyl)oxy]-7,8,9,10-tetrahydro-6,8,11-trihydroxy-8-(2-hydroxyacetyl)-1-methoxy-5,12-naphthacenedione
- 14-Hydroxydaunomycin
- 5,12-Naphthacenedione, 10-[(3-amino-2,3,6-trideoxy-α-L-lyxo-hexopyranosyl)oxy]-7,8,9,10-tetrahydro-6,8,11-trihydroxy-8-(hydroxyacetyl)-1-methoxy-, (8S-cis)-
- 5,12-Naphthacenedione, 10-[(3-amino-2,3,6-trideoxy-α-L-lyxo-hexopyranosyl)oxy]-7,8,9,10-tetrahydro-6,8,11-trihydroxy-8-(hydroxyacetyl)-1-methoxy-, (8S,10S)-

View More



Absolute stereochemistry shown

C₂₇H₂₉NO₁₁
5,12-Naphthacenedione, 10-[(3-amino-2,3,6-trideoxy-α-L-lyxo-hexopyranosyl)oxy]-7,8,9,10-tetrahydro-6,8,11-trihydroxy-8-(2-hydroxyacetyl)-1-methoxy-, (8S,10S)-

藥物情報資訊 (Drug Intelligence)

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: Farnitalia

INDICATIONS

[Ovarian cancer](#)
 Modality: Primary
 Highest Phase: Approved
[Source](#) ↗

[View All](#) →

PRIMARY TARGET

[DNA topoisomerase II](#)
 Function: Inhibitor
 Measurement: IC50 2.67 µM
[Source](#)

[View All](#) →

Targets ✕ [View Related Drugs](#)

Primary Target	相關靶標	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 關 適 應 症 所 處 臨 床 階 段 和 獲 批 資 訊 ✕

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 (7.1).

RECENT MAJOR CHANGES
 Contraindications, Nursing Mothers (4) Removed 8/2012
 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)
- Multiple Myeloma (1.3)

 After failure of prior systemic chemotherapy or intolerance to such therapy.

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

- INDICATIONS AND USAGE
 - Ovarian Cancer
 - AIDS-Related Kaposi's Sarcoma
 - Multiple Myeloma
- DOSAGE AND ADMINISTRATION
 - Usage and Administration Precautions
 - Patients With Ovarian Cancer
 - Patients With AIDS-Related Kaposi's Sarcoma
 - Patients With Multiple Myeloma
- ADVERSE REACTIONS
 - Overall Adverse Reactions Profile
 - Adverse Reactions in Clinical Trials
 - Post Marketing Experience
- DRUG INTERACTIONS
- USE IN SPECIFIC POPULATIONS
 - Pregnancy
 - Nursing Mothers
 - Pediatric Use
 - Geriatric Use
 - Hepatic Impairment
- OVERDOSAGE
- DESCRIPTION
- CLINICAL PHARMACOLOGY

CONTRAINDICATIONS
 Hypersensitivity reactions to a conventional formulation of doxorubicin HCl or the components of DOXIL (4.5.2)

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).

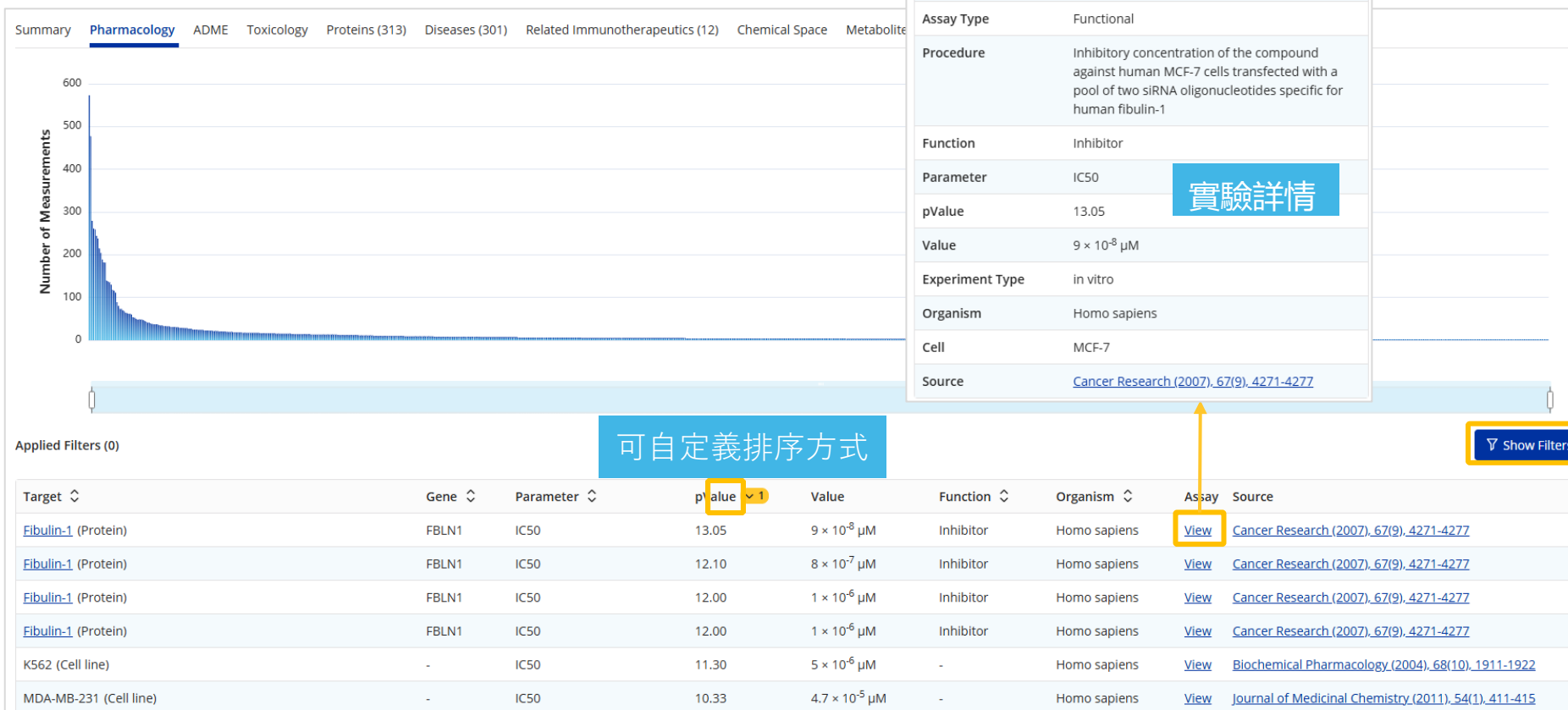
To report SUSPECTED ADVERSE REACTIONS contact Janssen Products, LP at 1-800-JANSSEN (1-800-326-7736) or FDA at 1-800-FDA-1088 or www.fda.gov/medwatch.

DRUG INTERACTIONS
 DOXIL may formulations
 DOXIL can
 Discontinue

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

FDA文件的pdf

配體藥理學資訊



← 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

實驗詳情

藥理活性實驗數據篩選項

Filters

- Chemical Filters
- pValue
- Biological Filters
 - Target 靶点
 - Target Type 靶点类型
 - Disease 疾病
 - Organism 生物有機體
 - Parameter 藥理學參數
 - Function 功能
 - Experiment Type 實驗類型
- Source Filters
- Document Type
- Publication Year
- Language

Organism

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

[View All](#)

Parameter

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

[View All](#)

Function

- Inhibitor
- Modulator
- Binder
- Substrate
- Antagonist

[View All](#)

配體ADME信息

ADME實驗數據篩選項

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

Predicted Properties

logP* - Partition Coefficient	logS - Solubility	logBB - Blood-Brain Barrier Permeability	Polar surface area (Å²)*	Plasma protein binding	Permeability glycoprotein	* Calculated using Advanced Chemistry Development Software (© 1994-2025 ACD/Labs)
0.918	-3.27	-1.96	206.07	67.32	1	

Applied Filters (0)

Parameter [^] 1	Value	Organism [^]	Assay	Source
t1/2	9.63 hr	Rattus	View	International Journal of Pharmaceutics (Amsterdam, Netherlands)(2019), 557(0), 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	Antonie van Leeuwenhoek International Journal of Microbiology (Amsterdam, Netherlands)(2019), 115(1), 2004385
t1/2	5.7 hr	Mus	View	World Journal of Microbiology (Singapore)(2013), 5(1), 06824 A1 2013-07-18
t1/2	11.9 hr	Mus musculus	View	International Journal of Pharmaceutics (Amsterdam, Netherlands)(2023), 528(1), 273-285
t1/2	17.9 hr	Rattus	View	Biochemical Pharmacology (Amsterdam, Netherlands)(2017), 94(4), 4279-4288
t1/2	3.5 hr		View	International Journal of Pharmaceutics (Amsterdam, Netherlands)(2017), 526(1-2), 443-454
t1/2	0.8 hr		View	AAAPS International Journal of Pharmaceutics (Amsterdam, Netherlands)(2017), 526(1-2), 443-454
t1/2	15.9 hr		View	Antonie van Leeuwenhoek International Journal of Microbiology (Amsterdam, Netherlands)(2017), 94(4), 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(0), 264-272

實驗詳情

Filters

Biological Filters

生物有機體

- Mus
- Rattus
- Homo sapiens
- Rattus norvegicus
- Macaca mulatta

[View All](#) [Apply](#)

Parameter

代謝相關參數

- t1/2
- Cmax
- AUC
- CL
- Vd

[View All](#) [Apply](#)

Experiment Type

實驗類型

- in vivo
- in vitro

[Apply](#)

Source Filters

- Document Type
- Publication Year
- Language

[Show Filters](#) [Download](#)

配體毒理學資訊

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

Applied Filters (0)

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- Vo
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- Vo
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

← Prev 1 2 3 4 5 ... 80 Next → Show 10 per page

← Prev (1 of 796) Next →

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 × 10 ⁴ μM
Disease	Cancer
Experiment Type	in vivo
Organism	Mus musculus
Source	Journal of Medicinal Chemistry (2003), 46(14), 2985-3007

實驗詳情

毒理學實驗數據篩選項

Biological Filters

Organism

- Homo sapiens
- Mus musculus
- Rattus norvegicus
- Mus
- Artemia salina

生物有機體

Parameter

- LC50
- IC50
- LD50
- MTD
- LDLo

毒理學參數

Experiment Type

- in vitro
- in vivo

實驗類型

Route of Administration

- Intraperitoneal
- Intravenous
- Oral
- Immersion
- Subcutaneous

給藥方式

Source Filters

Document Type

Publication Year

Language

Show Filters

配體相關靶點與疾病資訊

基於CAS數據關聯，一鍵關聯到該配體相關靶點與疾病資訊詳情頁，並探索更多關聯資訊

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)

View: List Sort: Relevance [View all associated proteins](#)

Protein	Organism	Count
1 KDR Vascular endothelial growth factor receptor 2	-	34K 486
2 EGFR Epidermal growth factor receptor	-	40K 460
3 KDR Vascular endothelial growth factor receptor 2	Homo sapiens	31K 332
4 SRC Proto-oncogene tyrosine-protein kinase Src	-	18K 418
5 CYP3A4 Cytochrome P450 3A4	Homo sapiens	10K 456

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

[Diseases](#) [Adverse Events](#) **副作用**

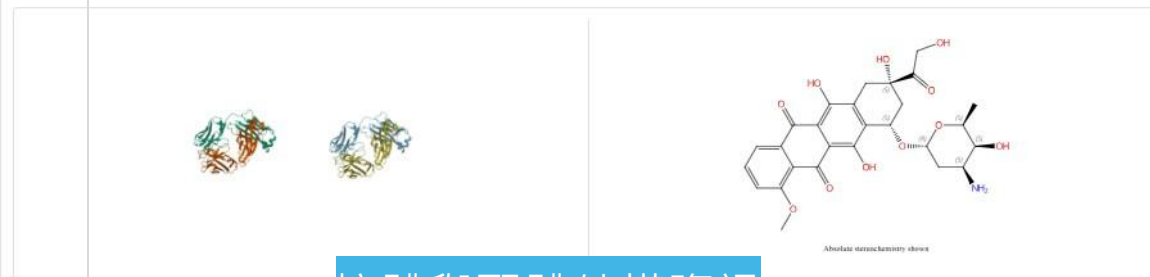
Sort: Relevance [View all associated diseases](#)

Disease	Description	Biomarkers	Count
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, Iset 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

配體相關免疫療法資訊

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

MAb-DMBA-SIL-Dox

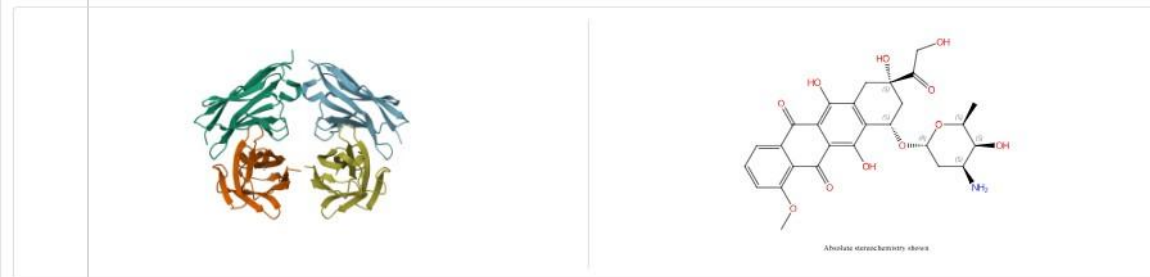


抗體與配體結構資訊

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 thiomaleimide Michael addition.

免疫療法詳情

Trastuzumab-PC4AP-DOX



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藥物詳情

Trastuzumab emtansine

CAS Registry Number: 1018448-65-1

1,972

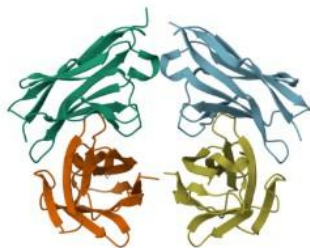
8

Retrosynthesis

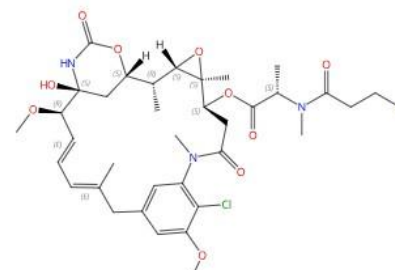
Predictive Analytics

...

Summary Pharmacology ADME Proteins (2) Diseases (1)



抗體3D結構圖



藥物分子結構

CAS DRUG INTELLIGENCE 藥物情報資訊

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

Heavy Chain Sequence

EVQLVESGGGLVQPGGSLRLSCAASGGFNIKDTYIHWRQAPGKGLEWVARIYPTNGYTRYADSVKGRFTISADTSKNTAYLQMNSLRAEDTAVVYSRWGGDG
FYAMDYDYWGQGLTVTVSSASTKGPSVFPLAPSSKSTSGGTAALGCLVKDYFPEPVTVSWNSGALTSVHTFPAVLQSSGLYSLSSVTVPSSSLGTQTYICNV
NHKPSNTKVDKKEPKSCDKTHTCPPCPAPELLGGPSVFLFPPKPKDTLMISRTPEVTCVVDVSHEDPEVKFNWYVDGVEVHNAKTKPREEQYNSTYRVVSVL
TVLHQDWLNGKEYKCKVSNKALPAPIEKTISKAKGQPREPQVYTLPPSREEMTKNQVSLTCLVKGFYPSDIAVEWESNGQPENNYKTPPVLDSDGSFFLYSKL
TVDKSRWQQGNVFSQVMHEALHNHYTQKSLSLSPGK

Light Chain Sequence

DIQMTQSPSSLSASVGVDRVITCRASQDVNTAAVAWYQQKPKAPKLLIYSASFYSGVPSRFSGSRTDFTLTISLQPEDFATYYQQHYTTPPTPTFGQG
TKVEIKRTVAAPSVFIFPPSDEQLKSGTASVVCLLNNFYPREAKVQWKVDNALQSGNSQESVTEQDSKDSYSLSSLTLSKADYEEKHKVYACEVTHQGLSSPV
TKSFNRGEC

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

CDR序列

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藥物詳情

相似配體結構與可視化分析

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

3D X-Axis logP Y-Axis Molecular Weight Z-Axis logS Similar Ligands

參數可選的二維/三維化學空間圖

相似配體結構

Similar Ligands (764)

- Hydrogen Bond Acceptors
- Hydrogen Bond Donors
- Freely Rotatable Bonds
- Molecular Weight
- Molar Refractivity
- Number of Atoms
- logP
- logS
- logBB
- PGP
- PSA
- PPB

98632-73-6 (1.00)
(8S,10R)-10-[(3-Amino-2,3,6-trideoxy- α -L-xylo-hexopyranosyl)oxy]-7,8,9,10-tetrahydro-5,12-naphthacenedione

79390-76-4 (1.00)
5,12-Naphthacenedione, 10-[(3-amino-2,3,6-trideoxy- α -L-xylo-hexopyranosyl)oxy]-7...

2170020-83-2
(8S,10S)-10-[(3-Amino-2,3,6-trideoxy- α -L-xylo-hexopyranosyl)oxy]-7,8,9,10-tetrahydro-5,12-naphthacenedione

56420-45-2 (1.00)
Epirubicin

76035-78-4 (1.00)
5,12-Naphthacenedione, 10-[(3-amino-2,3,6-trideoxy- α -L-xylo-hexopyranosyl)oxy]-7...

57819-79-1 (1.00)
5,12-Naphthacenedione, 10-[(3-amino-2,3,6-trideoxy- β -L-xylo-hexopyranosyl)oxy]-7...

55945-22-7
logP*: 5.560
Molecular Weight: 1173.34 g/mol
logS: -6.31

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

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探索配體代謝產物

已知代謝產物：Known
預測代謝產物：Confidence Score置信度分值，
表示發生該生物轉化的概率

Doxorubicin
CAS Registry Number: 23214-92-8

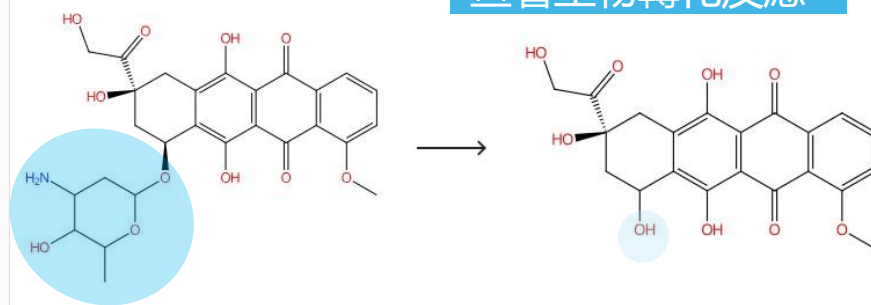
112K 1,642 Retrosynthesis Predictive Analytics

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

24385-10-2 Known 54193-28-1 Known 69417-09-0 Known

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

查看生物轉化反應



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

大綱

- CAS BioFinder簡介與檢界面介紹（介紹與介面）
- 配體檢索與配體詳情信息（配體與細節概述）
- **骨架檢索與構效關係分析（支架與搜救分析）**
- 蛋白/通路/靶點、疾病與生物標誌物（Proteins and Pathways; 疾病與生物標記）
- 生物活性預測（Predictive Analytics）

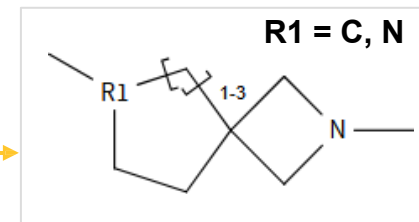
基於靶點或結構片段，探索活性結構骨架

Ligands **Scaffolds** Proteins Diseases

繪製核心結構片段

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

Draw a Structure



Filters
 Chemical Filters
 Rule of 5 Filter Preset
 ^ pValue
 1.70 to 13.00
 1.70 to 13.00
 Biological Filters
 Menin
 Cyclin E1-CDK2 complex
 Histone-lysine N-methyltransferase complex
 GTPase KRas
 Monoglyceride lipase
 View All

Scaffolds search for drawn structure
 2,649 Results

 Ligands: 210 Proteins: 9	 Ligands: 11 Proteins: 5	 Ligands: 55 Proteins: 1	 Ligands: 20 Proteins: 4
 Ligands: 34 Proteins: 1	 Ligands: 12 Proteins: 3	 Ligands: 8 Proteins: 12	 Ligands: 31 Proteins: 1
 Ligands: 1 Proteins: 1	 Ligands: 1 Proteins: 1	 Ligands: 1 Proteins: 1	 Ligands: 1 Proteins: 1

歸一化的活性

篩選關注的靶點

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

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

IC50越小，
pValue越大，
抑制活性越高。

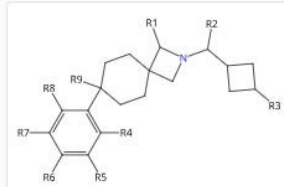
探索目標結構骨架的SAR數據

CAS BioFinder

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

Return to Results

Scaffold Summary



Associated Proteins
1

Filters

Chemical Filters

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

R-Groups

pValue

Druglikeness

ADME

Commercial Availability

Biological Filters

Target

Target Type

Disease

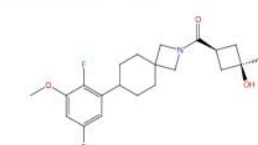
GIELXZVQJYHYPI-UHFFFAOYSA-N
Murcko scaffold InChI Key

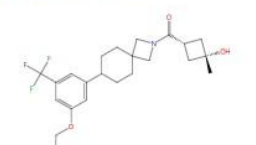
Ligands Pharmacology Similar Scaffolds

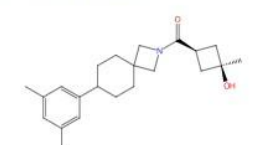
60 Results

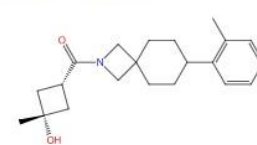
Sort: Relevance Get MMPA


Ligands: 60 Proteins: 1

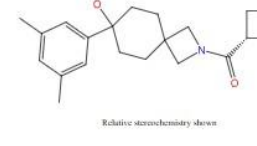
1 2765314-82-5 [7-(2,5-Difluoro-3-methoxyphenyl)-2-azaspiro[3.5]non-2-yl](*cis*-3-hydroxy-3-methy...

Metabolites: 4 Proteins: 1

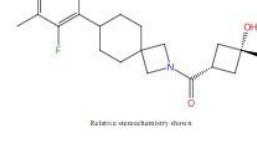
2 2765312-35-2 [7-[3-Ethoxy-5-(trifluoromethyl)phenyl]-2-azaspiro[3.5]non-2-yl](*cis*-3-hydroxy-3...

Metabolites: 4 Proteins: 1

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

Metabolites: 4 Proteins: 1

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

Metabolites: 7 Proteins: 1

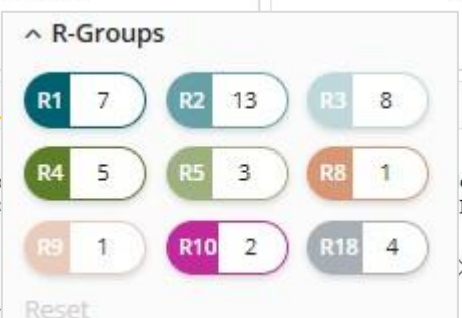
5 2765312-61-4 [7-[3-Ethyl-5-(trifluoro... non-2-yl)](*cis*-3-hydroxy...

Metabolites: 6 Proteins: 1

6 2765314-60-9 [7-(3,5-Dimethylphenyl)-7-methoxy-2-azaspiro[3.5]non-2-yl](*cis*-3-hydroxy-3-methy...

Metabolites: 6 Proteins: 1

7 2765314-68-7 [7-(2-Fluoro-3-methylphenyl)-2-azaspiro[3.5]non-2-yl](*cis*-3-hydroxy-3-methylcycl...

Metabolites: 5 Proteins: 1

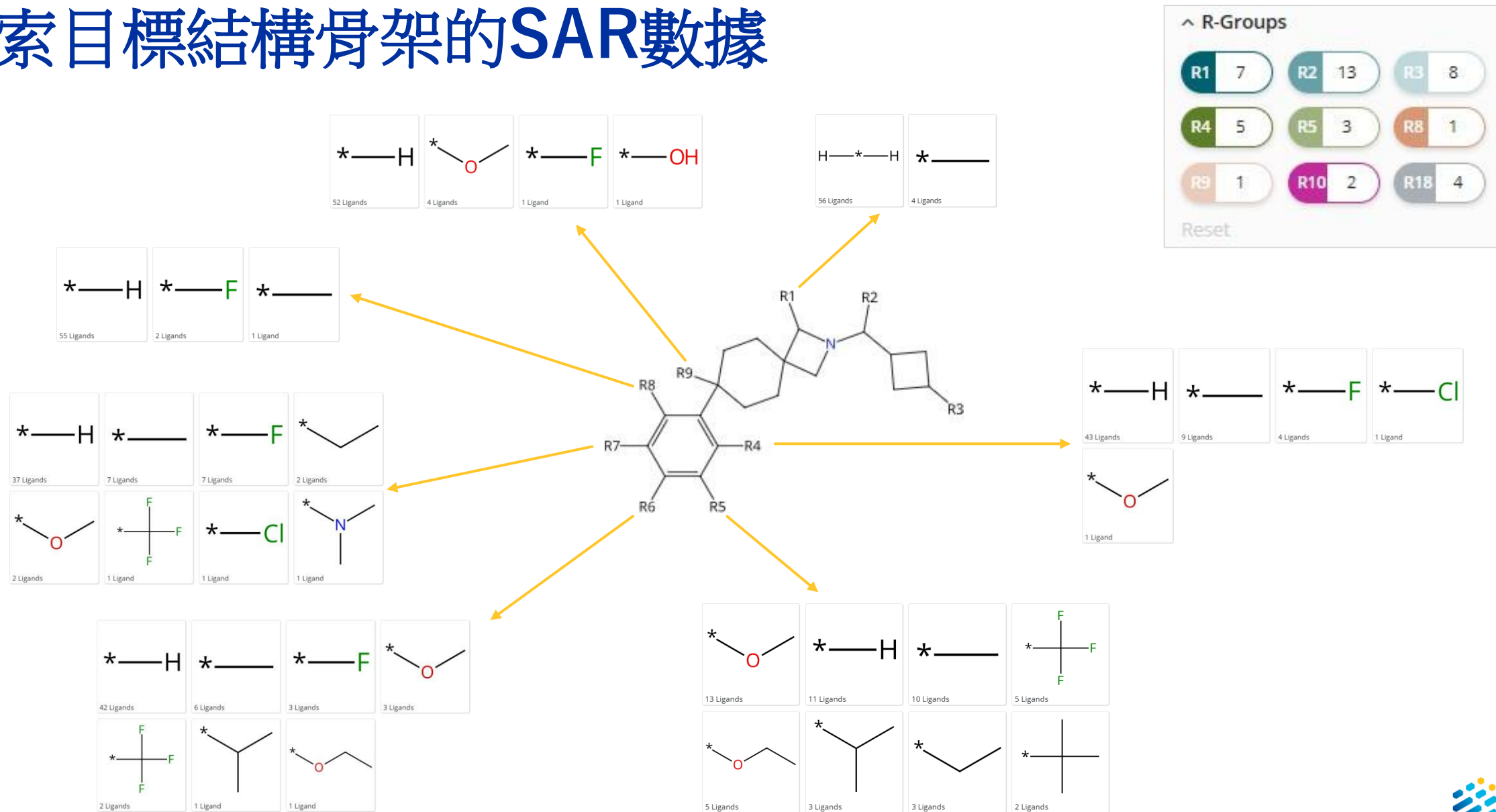
8

18



R-Group	Count
R1	7
R2	13
R3	8
R4	5
R5	3
R8	1
R9	1
R10	2
R18	4

探索目標結構骨架的SAR數據



符合分子對分析 (MMPA)

The screenshot displays the CAS MMPA web interface. At the top, the scaffold is identified as GIELXZVQJYHYPI-UHFFFAOYSA-N (Murcko scaffold InChI Key). The interface shows a list of results with chemical structures and names. A yellow box highlights the 'Get MMPA' button. Below the results, a dialog box titled 'Select a Target for Matched Molecular Pairs Analysis (MMPA)' is open, with 'Monoglyceride lipase' selected as the target. A blue box with the text '選擇目標靶點' (Select target) is overlaid on this dialog. To the right, another dialog box titled 'Select one R-Group Cluster to Visualize' is open, showing a grid of chemical structures. A blue box with the text '獲取目標R基團位點變化的MMPA活性對比結果' (Obtain MMPA activity comparison results for target R-group site changes) is overlaid on this dialog. A yellow arrow points from the 'Submit' button in the visualization dialog back to the 'Next' button in the target selection dialog.

Return to Results

Scaffold Summary

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...

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

選擇目標靶點

Select one R-Group Cluster to Visualize

15 Matched Molecular Pairs

10 Matched Molecular Pairs

10 Matched Molecular Pairs

10 Matched Molecular Pairs

獲取目標R基團位點變化的MMPA活性對比結果

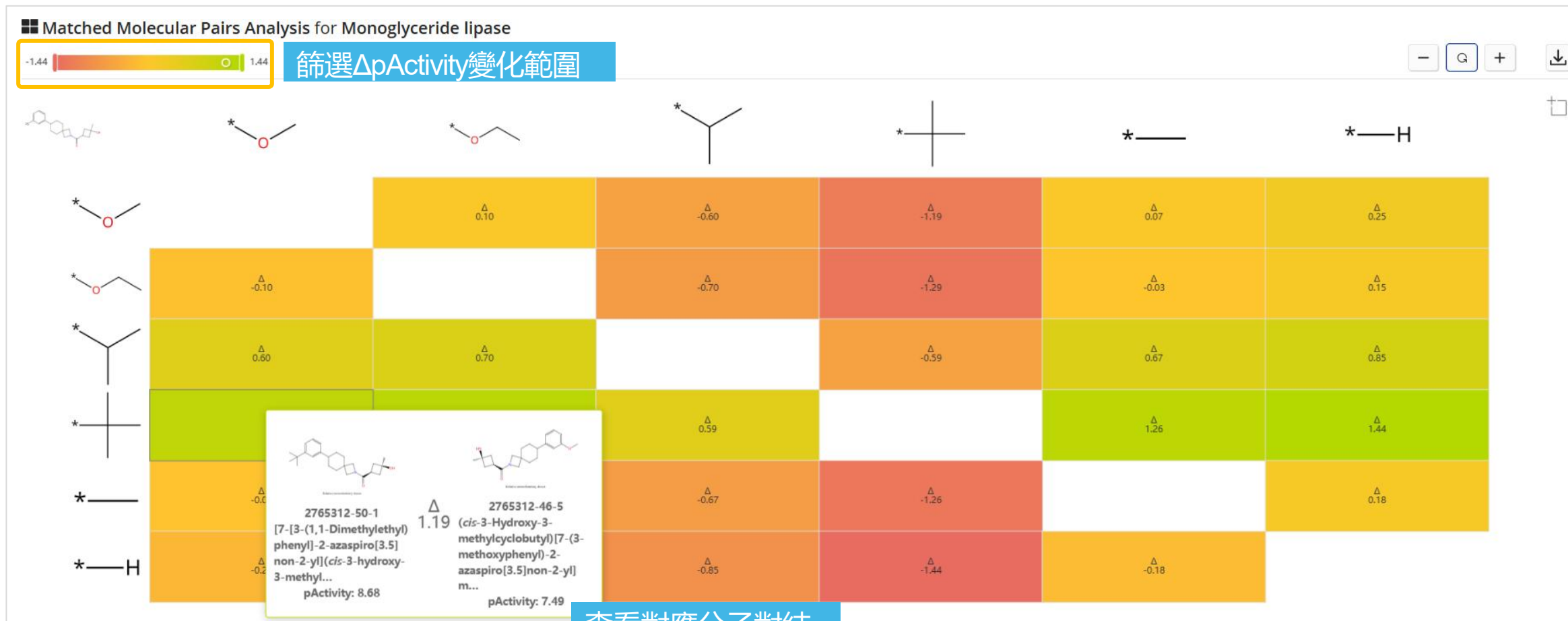
Show 100 per page

Previous **Submit** Cancel

Next Cancel

符合分子對分析 (MMPA)

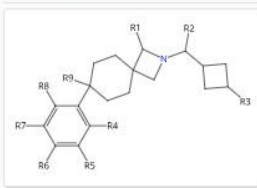
快速直觀獲取匹配分子對 $\Delta pActivity$ 熱圖



查看同一結構骨架中的配體藥理活性

← Return to Results

Scaffold Summary



Associated Proteins
1

Filters

Chemical Filters

Biological Filters

篩選關注靶點

Target

Monoglyceride lipase

Target Type

Disease

Organism

Parameter

Experiment Type


Source Filters

Document Type

Publication Year

GIELXZVQJYHYPI-UHFFFAOYSA-N
Murcko scaffold InChI Key

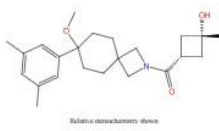
Ligands Pharmacology Similar Scaffolds



Assay Detail

← Prev (1 of 60) Next →

Ligand
2765314-60-9



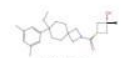

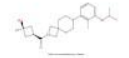
C₂₃H₃₃NO₃
[7-(3,5-Dimethylphenyl)-7-methoxy-2-azaspiro[3.5]non-2-yl]([cis-3-hydroxy-3-methy...

實驗詳情

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

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

Show Structures ON

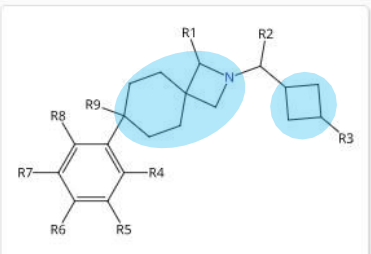
Ligand	Target	Gene	Parameter	pValue	Value	Function	Assay	Source
 2765314-60-9 [7-(3,5-Dimethylphenyl)-7-methoxy-2-azaspiro[3.5]non-2-yl]([cis-3-hydroxy-3-methy...	Monoglyceride lipase (Protein)	MGLL	IC50	9.08	8.4 × 10 ⁻⁴ μM	-	View	United States_US20220089538 A1 2022-03-24
 2765313-81-1 (cis-3-Hydroxy-3-methylcyclobutyl)[7-methoxy-7-[3-(1-methylethyl)phenyl]-2-az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

藥理活性數據

獲取與目標骨架相似骨架結構，啟發新的SAR假設

← [Return to Results](#)

Scaffold Summary



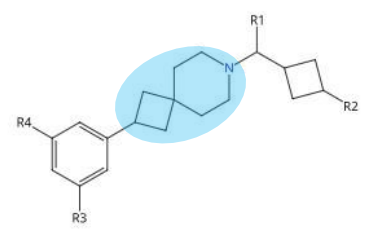
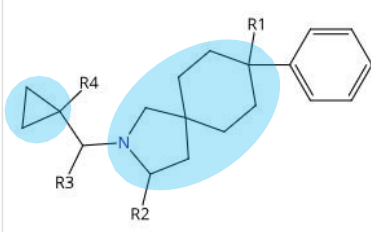
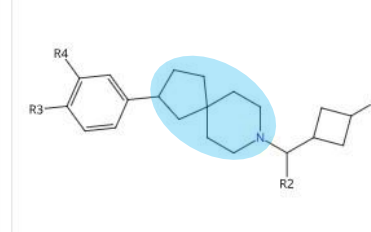
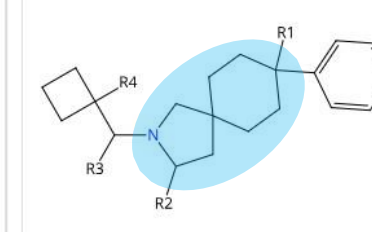
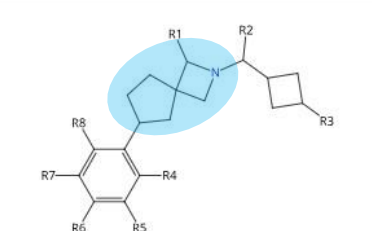
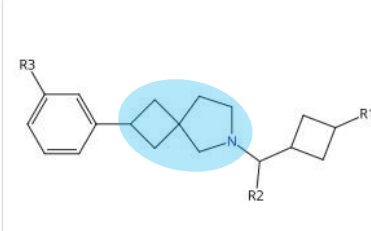
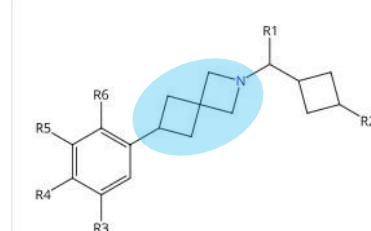
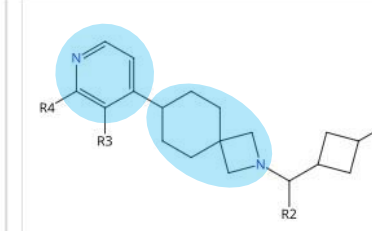
Associated Proteins
1

GIELXZVQYHYPI-UHFFFAOYSA-N
Murcko scaffold InChI Key

Ligands Pharmacology **Similar Scaffolds**

1,123 Scaffolds

獲取相似骨架結構(Similar Scaffolds) ;
基於相應藥效團的關鍵結構元素識別相似骨架結構

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

大綱

- CAS BioFinder簡介與檢界面介紹（介紹與介面）
- 配體檢索與配體詳情信息（配體與細節概述）
- 骨架檢索與構效關係分析（支架與搜救分析）
- **蛋白/通路/靶點、疾病與生物標誌物（Proteins and Pathways; 疾病與生物標記）**
- 生物活性預測（Predictive Analytics）

通過靶點、疾病或配體，獲取歸一化的蛋白檢索結果

CAS BioFinder

Proteins SYK 示例：SYK

Filters

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

Return to top

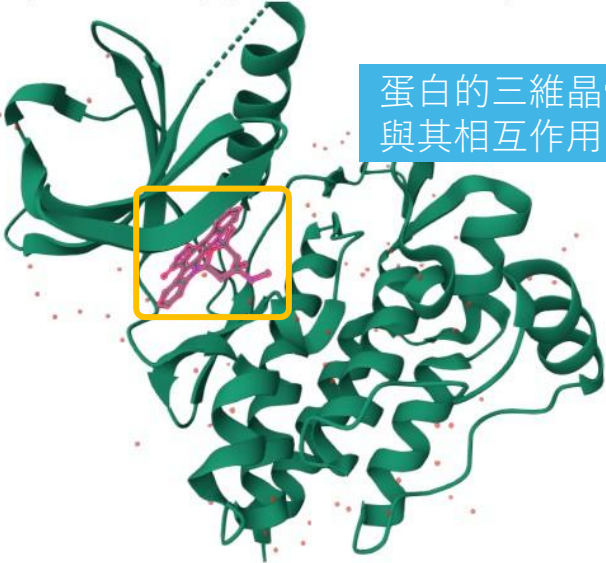
切換縮圖檢視或清單檢視

蛋白詳情資訊與立體結構展示

SYK
Tyrosine-protein kinase SYK

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

Crystal structure of the syk tyrosine kinase domain with Staurosporin



蛋白的三維晶體結構及與其相互作用的小分子

Organism: Homo sapiens, Rattus norvegicus, Mus musculus. 來源有機體

Sequence: >P43405-1|Tyrosine-protein kinase SYK|Homo sapiens
MASSGMADSANHLPPFFGNIITREEAEDYL VQGGMSDGLYLLRQSRNYLGGFALSVAHGRKAHHYI IERELNGTYAIAGGRTHASPADLCHYHSQESDGLVCLLKKPFNRPQGVQPK
TGPFDLKENLI IREYVQKTWMLQGQALEQAIISQKPQLEKLIATTAEHKMPWFHGKISREESEQIVLIGSKTNGKFLIRARDNNGSYALCLLHEGKVLHYRIDKDKTGLSIPGK
KFDLWQLVEHYSYKADGLLRVLTVPQCQKIGTQGNVNFGRPQLPGSHPATWSAGGISRIKSYSFPPKPGHRKSSPAQGNRQESTVSNFNPYEPAPWAADKGPQREALPMDTEVY
ESPYADPEEIRPKVYLDRLKLLTLEDKELGSGNFGTVKKGYYQMKVVKTVAVKILKNEANDPALDELLAEANVMQQLDNPIYIVRMIGICEAESWMLVMEAEGLNLYLQQR
HVKDKNIIELVHQVSMGMKYLEESNFVHRDLAARNVLLVTQHYAKISDFGLSKALRADENYYKAQTHGKWPVKWYAPEICINYYKFSKSDVWSFGVLMWEAFSYGQKPYRGMKGE
VTAMLEKGERMGCPCPREMYDLMLNLCWTYDVENRPGFAAVELRLRNYYDVVN

序列詳情

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](#)

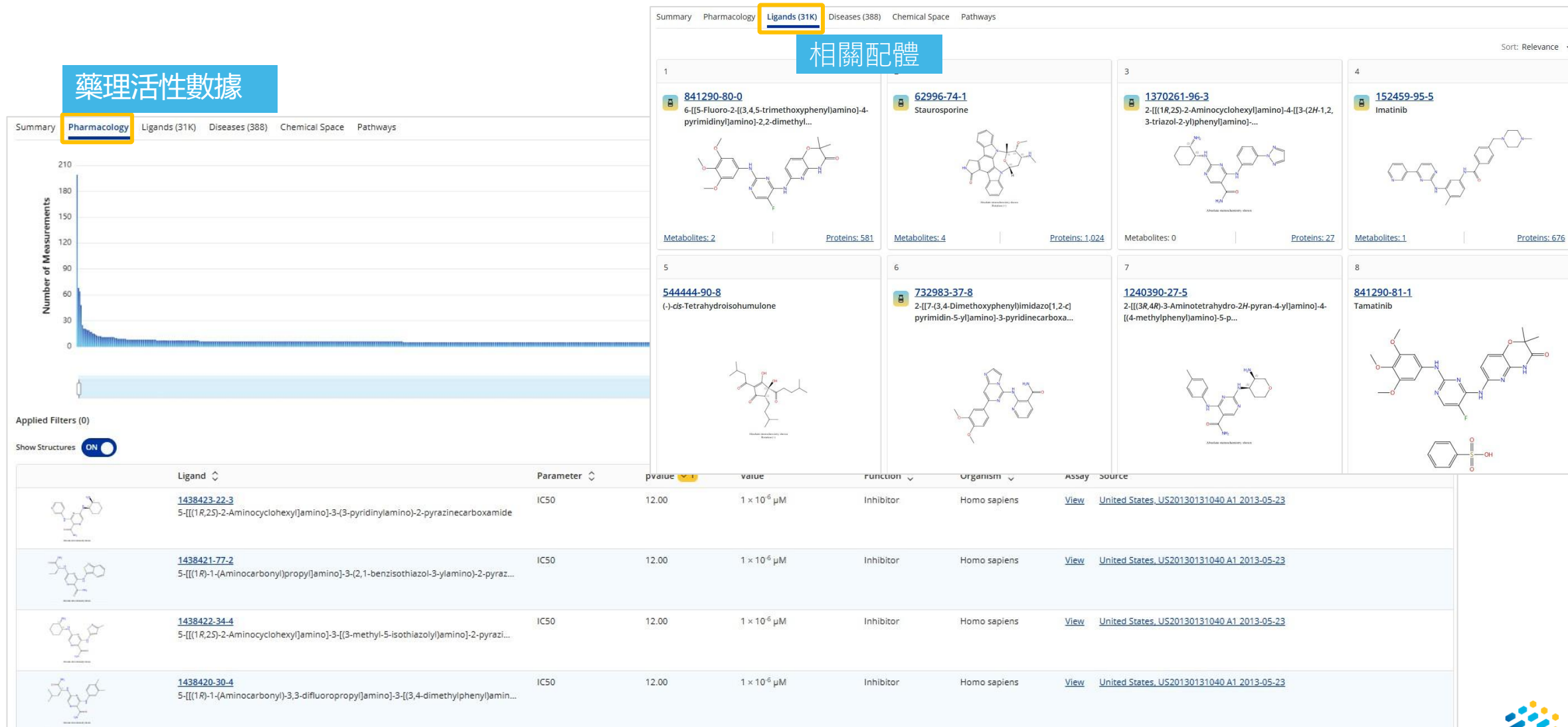
STAUROSPORINE
1XBC | Model 1 | Instance ASML_1 | B [auth A] | STU 1

1XBC [C] [+] [-] [Download] 下載cif格式結構檔


歸一化的靶點名稱
與其他詳情資訊

Synonyms
Spleen associated tyrosine kinase
Spleen tyrosine kinase

相關配體與藥理活性數據



蛋白相關疾病資訊




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	生物標誌物
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

蛋白的生物通路資訊



SYK
Tyrosine-protein kinase SYK

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

Pathway 通路	Reaction 作用詳情	Source 文獻來源
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	Coordinate interactions of Csk, Src, and Syk kinases with alpha IIb beta3 initiate integrin signaling to the cytoskeleton 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 (2001), 276(8), 5916-5923
	vasp + SLAP-130{p} + SLP-76{p} <=> vasp:SLAP-130{p}:SLP-76{p}	Journal of Biological Chemistry (2001), 276(8), 5916-5923
	Fibrinogen:(alpha IIb beta3)2:(Src{pY529})2 --	Journal of Biological Chemistry (1998), 273(48), 31890-31900
	VAV1{pY}:SLP-76{p}:Nck-1 + PAK1 + Rac1:GTP	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

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

By: Oberfell, Achim; Eto, Koji; Mocsal, 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 alpha IIb 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 alpha IIb 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 Cplplus and MEDLINE	Division of Vascular Biology, Department of Cell Biology The Scripps Research Institute La Jolla, California 92037 United States	Rockefeller University Press	English

一鍵連結到SciFinder文獻詳情頁

37

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通過疾病名稱、靶點或配體檢索相關疾病資訊

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

通過生物標誌物進行篩選

Diseases search for APP

Diseases

172 Results 疾病名稱

Sort: Relevance

Disease	Description	Biomarkers	生物標誌物	相關靶點與配體
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

疾病簡介

生物標誌物

相關靶點與配體

疾病詳情頁與相關藥物資訊

Alzheimer's disease

相關生物標誌物、藥理活性數據、配體與靶點

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.

疾病簡介

Synonyms

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

歸一化的疾病
同義詞清單

[View Less](#) ^

External Links and Identifiers

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

AI Drug Intelligence Summarization

AI總結藥物情報資訊

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

藥物情報資訊清單

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> -(4 <i>aR</i> ,6 <i>S</i> ,8 <i>aR</i>)-4 <i>a</i> ,5,9,10,11,12-Hexahydro-3-methoxy-11-methyl-6 <i>H</i> -benzofuro[3 <i>a</i> ,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 🔗

疾病與生物標誌物

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總結

Alzheimer's disease

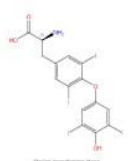
Summary **Biomarkers** Pharmacology Ligands (722K) Proteins (4,974)

Apply **生物標誌物** 參數 實驗說明 有機體 文獻來源 Show Filters Summarize Download

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 (1), 30(6), 567-76
(+)-Aldosterone	-	Pharmacodynamic/resp					Health Evaluation in African Americans Using RAS Therapy
(25S)-26-Hydroxycholesterol	-	Prognostic					Brain Communications (2023), 5(5), 1-14
[Pyruvate dehydrogenase (acetyl-transferring)] kinase isozyme 1, mitochondrial	-	Diagnostic					Journal of Biological Chemistry (2012), 287(44), 37245-37258

(-)-Thyroxine Detail

Biomarker
[51-48-9](#)



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 \(1\), 30\(6\), 567-76](#)

實驗詳情

大綱

- CAS BioFinder簡介與檢界面介紹（介紹與介面）
- 配體檢索與配體詳情信息（配體與細節概述）
- 骨架檢索與構效關係分析（支架與搜救分析）
- 蛋白/通路/靶點、疾病與生物標誌物（Proteins and Pathways; 疾病與生物標記）
- 生物活性預測（**Predictive Analytics**）

Predictive Analytics : 通過演算法預測配體對不同靶點的生物活性數據

Ligands Scaffolds Proteins Diseases

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

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

History (405) Predictive Sets (24)

Create New Set Panels

Predictive Test XXX
CAS Full Pharmacology (Default) - Complete

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

Updated on 29 August 2025

Rerun analysis for set
Add ligands from file
Edit set
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

選擇不同的預測面板

上傳.sdf文件

可從檢索結果集中添加配體結構

Filters

Chemical Filters

Rule of 5 Filter Preset
OFF 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 Scaffolds Pharmacology

25 of 9,190 Selected

Sort: Relevance Predictive Analytics

1
1961259-82-4
2,5-Diamino-1-(4-methylphenyl)-1H-pyrrole-3,4-dicarboxaldehyde

2
1961259-76-6
2,5-Diazo-1-(4-methylphenyl)-1H-pyrrole-3,4-dicarboxaldehyde

3
2270167-74-1
(3R,4R)-4-Methyl-1-(8-methyl-5-quinoliny)-3-pyrrolidinamine

4
2002854-95-5
4-(3-Hydroxy-3-methyl-1-pyrrolidinyl)-3-methylbenzotrile

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

7
1067895-50-4
8-Cyclobutyl-2-[4-(1-methyl-1H-pyrazol-4-yl)phenyl]-2,8-diazaspiro[4.5]decane

Metabolites: 2 Proteins: 0

Metabolites: 2 Proteins: 0

Metabolites: 4 Proteins: 2

Metabolites: 2 Proteins: 0

Metabolites: 2 Proteins: 0

Absolute stereochemistry shown

Absolute stereochemistry shown

Absolute stereochemistry shown

Absolute stereochemistry shown

Absolute stereochemistry shown

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

不同的蛋白靶點面板說明

History (407) Predictive Sets (25)

Create New Set Panels

Predictive Set CAS Breast Cancer Screen

Ligands: 25

Updated on 09 September

+ Create New Panel

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

自訂靶點面板

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	
CAS B...	
CAS M...	

Targets to Include in Panel **可自定义面板名称**

Create Predictive Analytics Panel

Panel Name
Predictive_Panel_Test

Description (Optional)

Cancel **Create Panel**

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

← Prev 1 2 3 4 5 ... 118 Next → Show 25 per page

Selected Targets

- Prostaglandin F2-alpha receptor (Felis catus) X
- Gag-pol polyprotein (Escherichia coli) X
- Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform (Rattus norvegicus) X
- Dihydroorotate dehydrogenase (quinone) (Plasmodium falciparum Dd2) X
- Bifunctional dihydrofolate reductase-thymidylate synthase (Cryptosporidium hominis) X

Cancel **Save**

生物活性預測結果

← Return to Predictive Analytics

Predictive_Set_09_09_2025_1002

Set Summary

Rerun Set Analysis
Complete - Last ran 09 Sep 2025

CAS Breast Cancer Screen

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](#)

Ligands Pharmacology

Show Structures

可直接連結到相關靶點詳情頁

從左到右涉及的方法有：
MLM, SAS, SEA, SIM, XPI

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	●●●●●

使用左側篩選功能可對這些數據進行細化分析：

- 活性值(pActivity)
- 置信度分數(Confidence score)
- 靶點(Target)
- 有機體(Organism)

助於探索特定範圍內的pAct, 或有較高可信度的預測資訊。

總結

配體檢索 (Ligands)

- 基於藥物名稱、CAS RN、結構、靶點、疾病等，獲取配體資訊
- 通過類藥性、ADME、實驗參數、藥物功能、生物有機體等，進行篩選聚焦
- 查看並評估化合物的藥理學、ADME、毒理學和代謝物資訊及可視化展示

骨架檢索(Scaffolds)

- 基於結構或靶點等資訊，高效獲取相關骨架結構，並通過官能團R-Groups，進行構效關係分析
- 通過 SAR 以及MMPA，優化目標骨架或先導化合物的效力和選擇性
- 探索針對關注靶點同一結構骨架中活性最高的配體，獲取相似骨架結構與拓展

蛋白/通路/靶點與疾病檢索(Proteins & Diseases)

- 高效獲取蛋白質通路/靶點與疾病生物標誌物資訊，探索藥物作用機制和適應症

預測配體 與不同靶點的生物活性(Predictive Analytics)

- 預測特定結構針對特定靶點的藥理活性資訊
- 關注配體的脫靶效應與藥物再利用

相關資源 Learn More

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

獲取CAS BioFinder登錄訪問網址

<https://www.cas.org/solutions/biofinder-discovery-platform>

瞭解更多關於CAS BioFinder的資訊

<https://cas-biofinder.zendesk.com/hc/en-us>

獲取CAS BioFinder使用說明資訊

獲取更多技術支援與說明，請聯繫：tliu2@acs-i.org

Between problems
and progress **are**
connections that
matter

謝謝！

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