

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

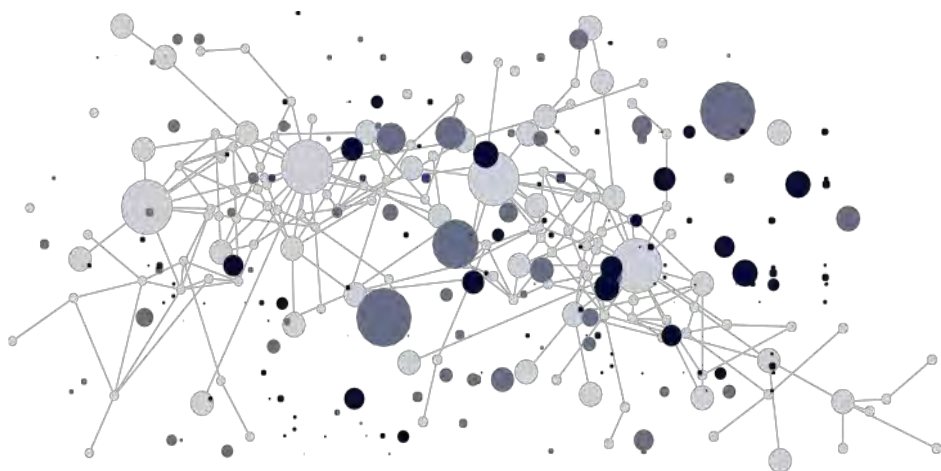
- 信息鴻溝會導致創新管線薄弱、研發效率低下，以及意外的知識產權風險
- 由於數據量和數據類型日益複雜，藥物發現流程中，整合和分析關鍵的研發數據資訊，對於迅速做出關鍵決策至關重要。
- 持續的數據管理有助於開發差異化的成果，支撐創新藥物的發現，確保藥物研發成功進入審批階段，並可避免後續智慧財產權問題。

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

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/

BTKh

BTK Orange II

BTK Black 10BX

BTK Victoria Blue

BTK deficiency

自動提示敘詞表

CAS BioFinder

Ligands BTK

Draw

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

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

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-

藥物情報信息標識

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

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

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

Reset Filter

Chemical Filters

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

pValue
2 to 13
2 to 10

Modality
2 to 10
2 to 10

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

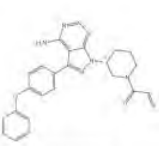
Ligands search for BTK

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

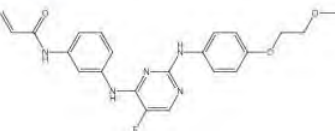
9,273 Results

936563-96-1
Ibrutinib



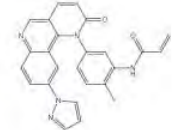
Metabolites: 3 | Proteins: 687

1202757-89-8
CC 292



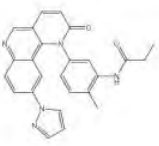
Metabolites: 7 | Proteins: 215

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



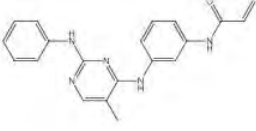
Metabolites: 7 | Proteins: 16

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



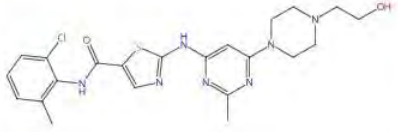
Metabolites: 8 | Proteins: 15

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



Metabolites: 12 | Proteins: 12

302962-49-8
Dasatinib



Metabolites: 4 | Proteins: 733

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



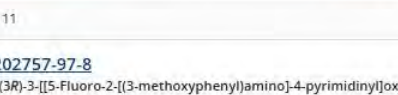
Metabolites: 8 | Proteins: 15

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



Metabolites: 12 | Proteins: 12

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

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CAS
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配體檢索結果的縱覽與聚焦

可通過檢索進行篩選聚焦

靶点

疾病

有機參數功能

實驗類型

Modality

- ☐ Small Molecule
- ☐ Protein/Peptide
- ☐ Other
- ☐ Coordination Compound
- ☐ Antibody
- ☐ Polymer
- ☐ Antibody Drug Conjugate

Approval Status

- ☐ Other
- ☐ Investigational
- ☐ US Approved
- ☐ Possibly Marketed Outside US
- ☐ Designated
- ☐ US Previously Marketed
- ☐ US Approved OTC

[View Fewer](#)

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



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

112K

1,642

Retrosynthesis

Predictive Analytics

...

View Associated Scaffold

View in CAS SciFinder

連結到CAS SciFinder

查看關聯資訊

Summary

Pharmacology

ADME

Toxicology

Proteins (313)

Diseases (301)

Related Immunotherapeutics (12)

Chemical Space

Metabolites (4)

Similar Ligands (764)

Absolute stereochemistry shown

$C_{27}H_{29}NO_{11}$

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)-

配體屬性資訊

H bond acceptors*	H bond donors*	Molecular weight (g/mol)	Molar refractivity (m ² /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)

Canonical SMILES

22 other names for this Ligand

配體相關信息標籤頁

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 All

View Related Drugs

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配體結構資訊與其他名稱

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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

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INDICATIONS

Ovarian cancer
Modality: Primary
Highest Phase: Approved
Source

PRIMARY TARGET

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

Targets

相關靶標

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

View All

View Related Drugs

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

WARNING: INTENSIVE REACTIONS, MYELOSUPPRESSION, CARDIOTOXICITY, LIVER IMPAIRMENT, SUBSTITUTION

RECENT MAJOR CHANGES

INDICATIONS AND USAGE

DOSAGE AND ADMINISTRATION

FULL PRESCRIBING INFORMATION: CONTENTS

ADVERSE REACTIONS

DRUG INTERACTIONS

USE IN SPECIFIC POPULATIONS

OVERDOSAGE

CLINICAL PHARMACOLOGY

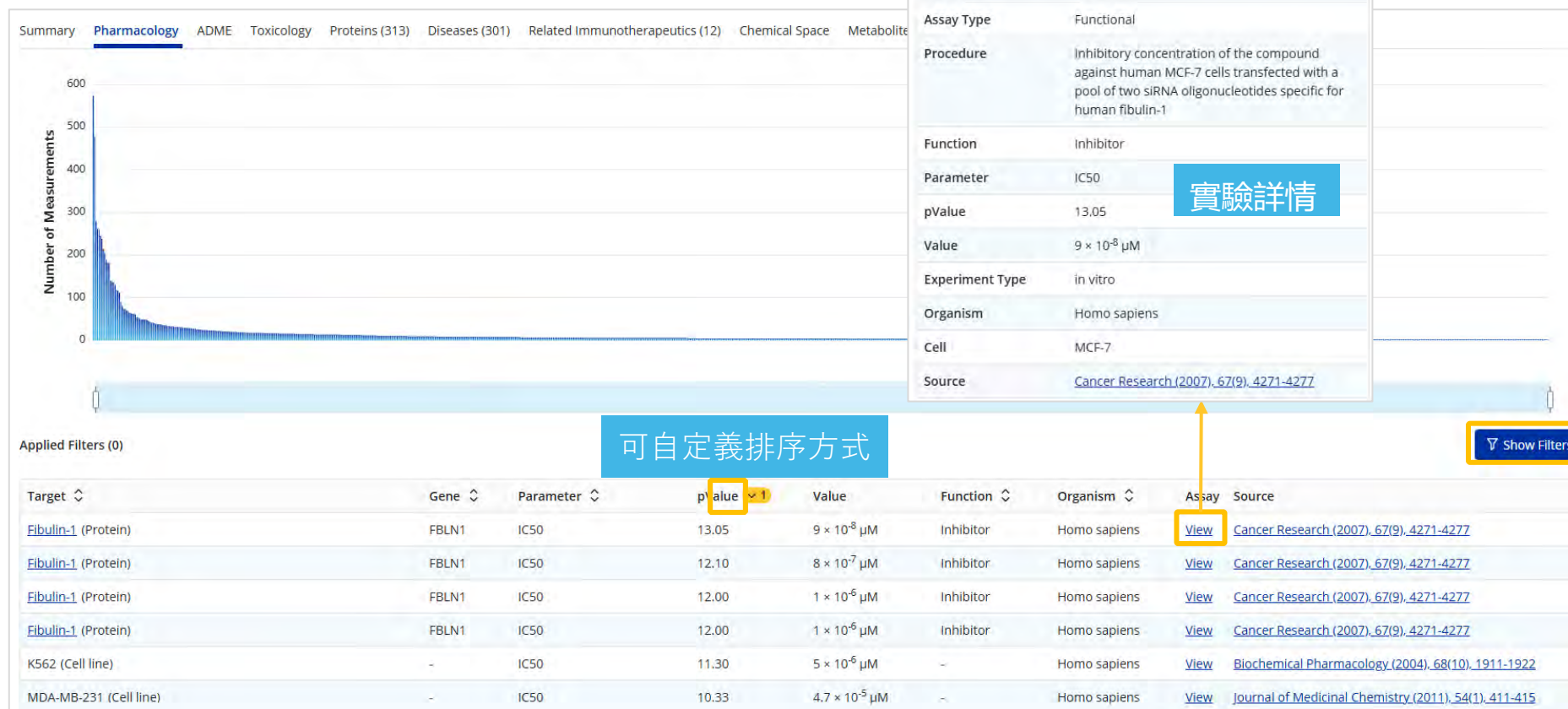
FDA文件的pdf

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配體藥理學資訊



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

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

Predicted Properties

logP* - Partition Coefficient

0.918

logS - Solubility

-3.27

logBB - Blood-Brain Barrier Permeability

-1.96

Polar surface area (Å²)*

206.07

Plasma protein binding

67.32

Permeability glycoprotein

1

* 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
t1/2	32 hr	Rattus	View	Journal of Pharmaceutical Sciences
t1/2	6.8 hr	Macaca mulatta	View	Anticancer Research
t1/2	5.7 hr	Mus	View	Advanced Drug Delivery Reviews
t1/2	11.9 hr	Mus musculus	View	World Journal of Pharmacy
t1/2	17.9 hr	Rattus	View	International Journal of Pharmaceutics
t1/2	3.5 hr		View	Biochemical Pharmacology
t1/2	0.8 hr		View	AAI
t1/2	15.9 hr		View	Anticancer Research
Vd	970.8667 L		View	International Journal of Pharmaceutics

← Prev

1

63

64

65

66

67

→

← 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(), 264-272

實驗詳情

ADME實驗數據篩選項

Filters

Biological Filters

Organism

☐ Mus

☐ Rattus

☐ Homo sapiens

☐ Rattus norvegicus

☐ Macaca mulatta

View All

Parameter

☐ t1/2

☐ Cmax

☐ AUC

☐ CL

☐ Vd

View All

Experiment Type

☐ in vivo

☐ in vitro

Source Filters

Document Type

Publication Year

Language

生物有機體

代謝相關參數

實驗類型

Show Filters

?

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 100 Pavia, Italy) V.44- 1989- Volume(issue)/page/year
IC50	4.8 mg/L	Mus musculus	View	JOET ... ck, Ireland) V.1- 1979- Volume(issue)/page/year

1 2 3 4 5 80 Next → Show 10 per page

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 × 10⁴ μM

Disease [Cancer](#)

Experiment Type in vivo

Organism Mus musculus

Source [Journal of Medicinal Chemistry \(2003\), 46\(14\), 2985-3007](#)

實驗詳情

Biological Filters

Organism

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

View All

Parameter

- ☐ LC50
- ☐ IC50
- ☐ LD50
- ☐ MTD
- ☐ LDLo

View All

Experiment Type

- ☐ in vitro
- ☐ in vivo

Route of Administration

- ☐ Intraperitoneal
- ☐ Intravenous
- ☐ Oral
- ☐ Immersion
- ☐ Subcutaneous

Source Filters

Document Type

Publication Year

Language

毒理學實驗數據篩選項

生物有機體

毒理學參數

實驗類型

給藥方式

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

⋮

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
6 FLT3 Receptor-type tyrosine-protein kinase FLT3	-
7 EGFR Epidermal growth factor receptor	-
8 CYP3A4 Cytochrome P450 3A4	-
9 PDGFRB Platelet-derived growth factor receptor beta	-
10 IGF1R Insulin-like growth factor receptor 1	-

DiseasesAdverse Events副作用

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

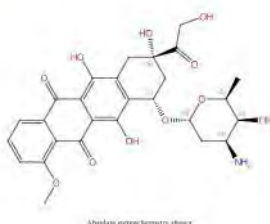
基於 ChEMBL 數據關聯，
配體相關靶點與疾病資訊詳情頁，
並探索更多關聯資訊

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)
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MAb-DMBA-SIL-Dox



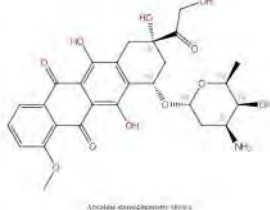


抗體與配體結構資訊

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 thiolmaleimide Michael addition.

Trastuzumab-PC4AP-DOX





抗體與配體結構資訊

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.

免疫療法詳情

ADC藥物詳情

Trastuzumab emtansine

CAS Registry Number: 1018448-65-1

1,972

8

Retrosynthesis

Predictive Analytics

...

Summary

Pharmacology

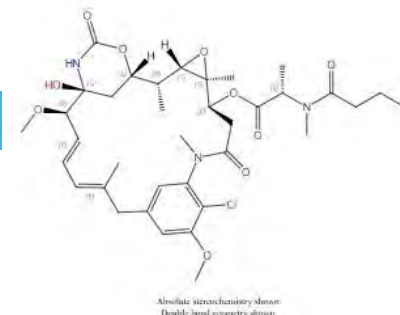
ADME

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

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](#)

Heavy Chain Sequence

EVQLVESGGGLVQPGGSLRLSCAASGGFNIKDITYIHWRQAPGKGLEWVARIYPINGYITRYADSVKGRFTISADTSKNTAYLQMNSLRAEDTAVVYSRWGGDGFYAMDYDYWGQGLTVTVSSASTKGPSVFPLAPSSKSTSGGTAALGCLVKDYFPEPTVSWNSGALTSVHTFPAVLQSSGLYSLSSVTVPSSSLGTQTYICNVNHKPSNTKVDKKVEPKSCDKTHTCPPCPAPELLGGPSVFLFPPKPKDTLMISRTPEVTCVVDVSHEDPEVKFNWYVDGVEVHNAKTKPREEQYNSTYRVVSVLTVLHQDWLNGKEYKCKVSNKALPAPIEKTISKAKGQPREPQVYTLPPSREEMTKNQVSLTCLVKGFYPSDIAVEWESNGQPENNYKTPPVLDSDGSFFLYSKLTVDKSRWQQGNVVFSCSVMEALHNHYTQKSLSLSPGK

Light Chain Sequence

DIQMTQSPSSLSASVGDRVTITCRASQDVNTAAVAWYQQKPKAPKLLIYSASFLYSGVPSRFSGSRSGTDFTLTISLQPEDFATYYQHYTTPPTPTFGQG TKVEIKRTVAAPSVFIFPPSDEQLKSGTASVVCLLNNFYPREAKVQWKVDNALQSGNSQESVTEQDSKDSYSTLSSTLTLSKADYEKHKVYACEVTHQGLSSPVTKSFNRGEC

重鏈/輕鏈序列

HCDR1
GFNIKDTY

HCDR2
IYPINGYT

HCDR3
SRWGGDGFYAMDY

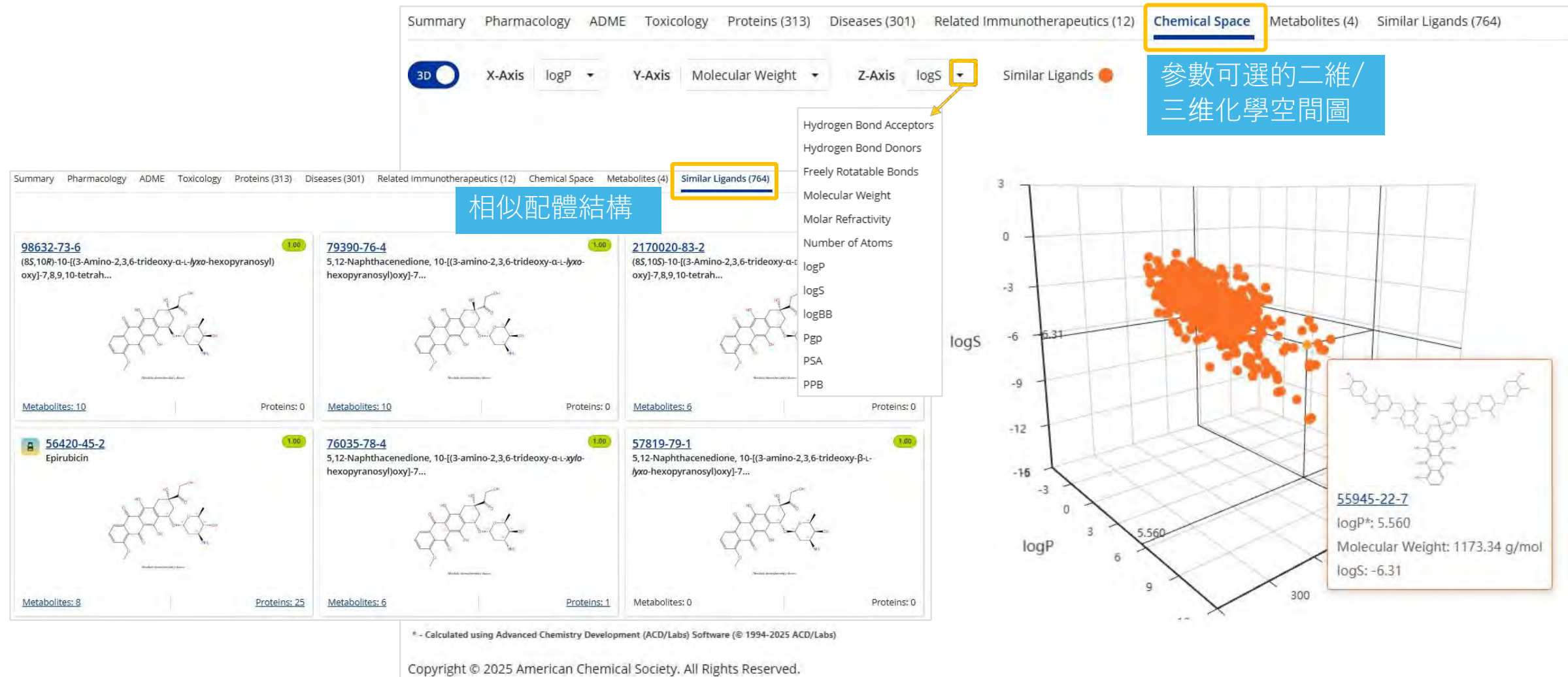
LCDR2
SAS

LCDR1
QDVNTA

LCDR3
QQHYTTPPT

CDR序列

相似配體結構與可視化分析



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

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）

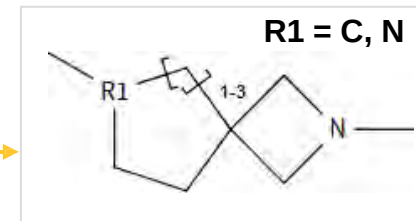
基於靶點或結構片段，探索活性結構骨架

Ligands **Scaffolds** Proteins Diseases

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

繪製核心結構片段

Draw a Structure



Filters

Chemical Filters

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

pValue
1.70 to 13.00

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: 1 Proteins: 1

11. Ligands: 1 Proteins: 1

12. Ligands: 1 Proteins: 1

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

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

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

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

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

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

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...

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

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

Metabolites: 4 Proteins: 1

Metabolites: 4 Proteins: 1

Metabolites: 4 Proteins: 1

Metabolites: 7 Proteins: 1

Metabolites: 6 Proteins: 1

Metabolites: 3 Proteins: 1

Metabolites: 6 Proteins: 1

Metabolites: 5 Proteins: 1

18

Ligands: 60 Proteins: 1

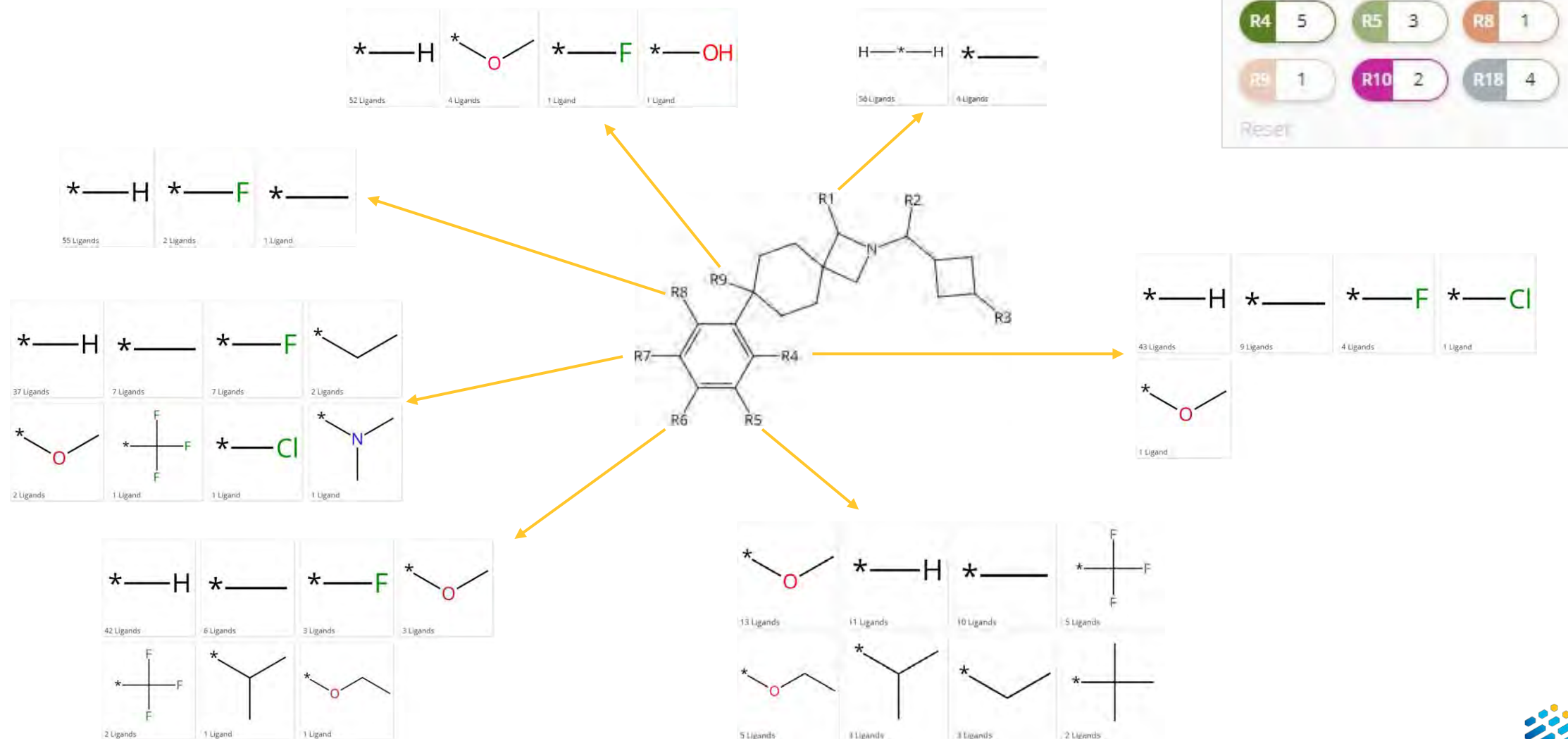
Sort: Relevance Get MMPA

R-Groups

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

Reset

探索目標結構骨架的SAR數據



符合分子對分析 (MMPA)

← [Return to Results](#)

Scaffold Summary

GIELXZVQJYHYPI-UHFFFAOYSA-N
Murcko scaffold InChI Key

Ligands Pharmacology Similar Scaffolds

60 Results

Sort: Relevance [Get MMPA](#)

1 2 3 4

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

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

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

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

[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

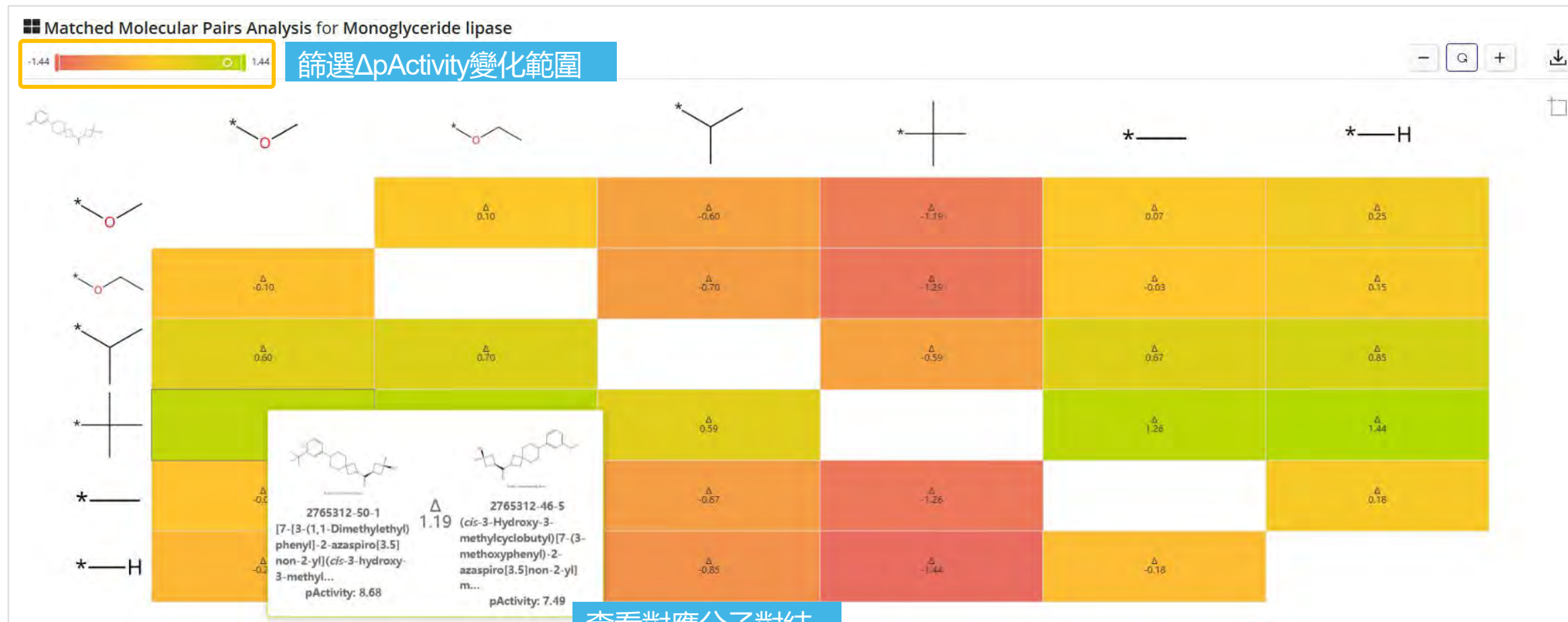
獲取目標R基團位點變化的MMPA活性對比結果

Show 100 per page

[Previous](#) [Submit](#) [Cancel](#)

符合分子對分析 (MMPA)

快速直觀獲取匹配分子對 $\Delta pActivity$ 熱圖



查看對應分子對結構資訊與pActivity

查看同一結構骨架中的配體藥理活性

← [Return to Results](#)

Scaffold Summary

GIELXZVQJYHYPI-UHFFFAOYSA-N
Murcko scaffold InChI Key

Ligands **Pharmacology** Similar Scaffolds

Number of Measurements

Associated Proteins
1

Filters

Chemical Filters

Biological Filters

Target

☒ Monoglyceride lipase

Target Type

Disease

Organism

Parameter

Experiment Type

Source Filters

Document Type

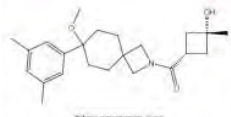
Publication Year

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

Show Structures ON

Assay Detail (1 of 60) Next →

Ligand
[2765314-60-9](#)



實驗詳情

Target: [Monoglyceride lipase \(Protein\)](#)

Gene: MGLL

Assay Type: Functional

Procedure: FAH assay

Parameter: IC50

pValue: 9.08

Value: $8.4 \times 10^{-4} \mu\text{M}$

Disease: [Disease of cellular proliferation](#)

Experiment Type: in vitro

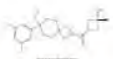
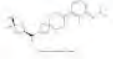
Organism: Homo sapiens

Cell: HeLa

Cell Detail: Cervical cancer cell

Source: [United States, US20220089538 A1 2022-03-24](#)

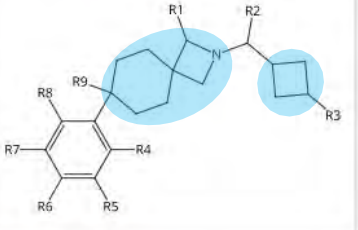
藥理活性數據

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-methyl-2-azaspiro[3.5]non-2-yl)]	Monoglyceride lipase (Protein)	MGLL	IC50	9.08	$8.4 \times 10^{-4} \mu\text{M}$	-	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

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

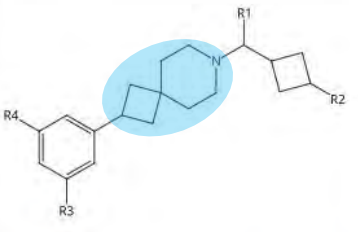
1

GIELXZVQYHYPI-UHFFFAOYSA-N
Murcko scaffold InChI Key

Ligands Pharmacology **Similar Scaffolds**

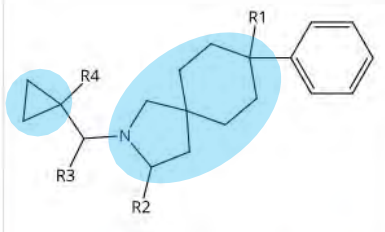
1,123 Scaffolds

1



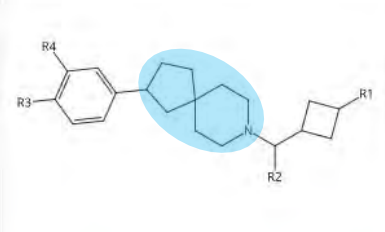
[Ligands: 2](#) | [Proteins: 1](#)

2



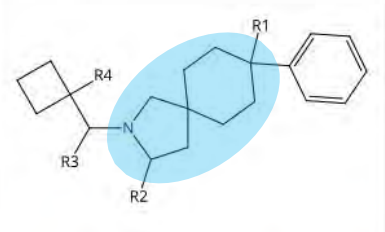
[Ligands: 9](#) | [Proteins: 2](#)

3



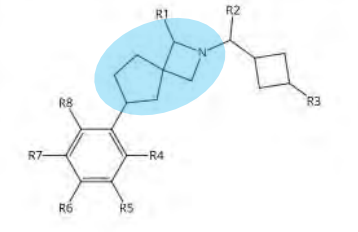
[Ligands: 3](#) | [Proteins: 1](#)

4



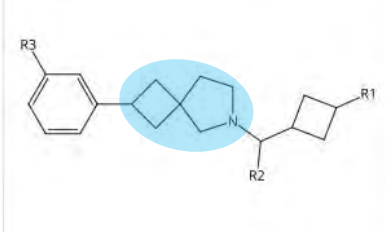
[Ligands: 9](#) | [Proteins: 2](#)

5



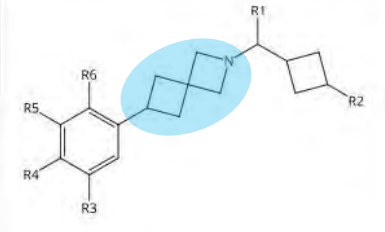
[Ligands: 69](#) | [Proteins: 1](#)

6



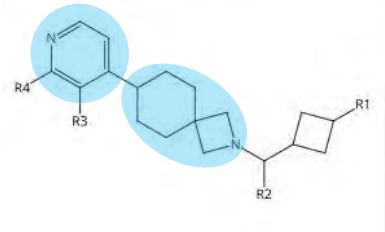
[Ligands: 1](#) | [Proteins: 1](#)

7



[Ligands: 9](#) | [Proteins: 1](#)

8



[Ligands: 2](#) | [Proteins: 1](#)

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

31

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CAS
A division of the
American Chemical Society

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

Biological Filters

Source Filters

Proteins search for SYK

Proteins Pharmacology

4 Results

Sort: Relevance View: Grid

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

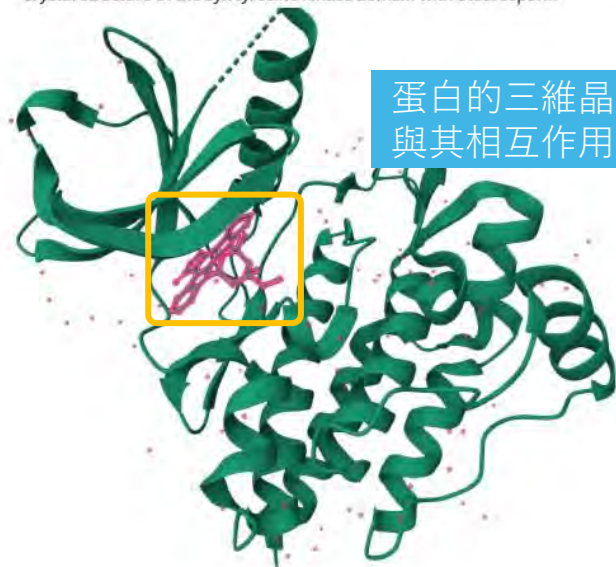
蛋白詳情資訊與立體結構展示

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

STAUSPORINE

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

1XBC

↺

+

-

↓

下載cif格式結構檔

Homo sapiens

unspecified

Rattus norvegicus

Mus musculus

來源有機體

Organism

Homo sapiens

GET FASTA

Copy Sequence

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

MASSGMADSANHLPPFFGNITREEAEDYLQGGMSDGLYLLRQSRNYLGGFALSVAHGRKAHHYIERELNGTYAAGGRTHASPADLCHYHSQESDGLVCLLKPPFNRPGVQPK
TGPFDLKENLIREYKQTWNLQGALEQAIISQKPQLEKIATTAHEKMPWFHGKISREESEQIVLIGSKTNGKFLIRARDNNGSYALCLLHEGKVLHYRIDKDKTGLSIPGK
KFDTLWQLVEHYSYKADGLLRVLTPCQKIGTQGNVNFGRPQLPGSHPATWSAGGIISRIKSYSPKPGHRKSSPAQGNRQESTVSFNPEPELAPWAADKGPQREALPMDTEVY
ESPYADPEEIRPKVYLDRKLLTLEDELGSGNFGTVKKGYQMKVVKTVAVKILKNEANDPALKDELLAEANVMQQLDNPIYIRMIIGICEAESWMLVMEAEGLPLNKYLQQR
HVKDKNIIELVHQVSMGMKYLEESNFVHRDLAARNVLLVTQHYAKISDFGLSKALRADENYYKAQTHGKWPVKWYAPECINYYKFSKSDVWSFGVLMWEAFSYGQKPYRGMKGSE
VTAMLEKGERMGCPCAGCPREMYDLMLNLCTYDVENRPGFAAVELRLNYYDVVN

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](#)

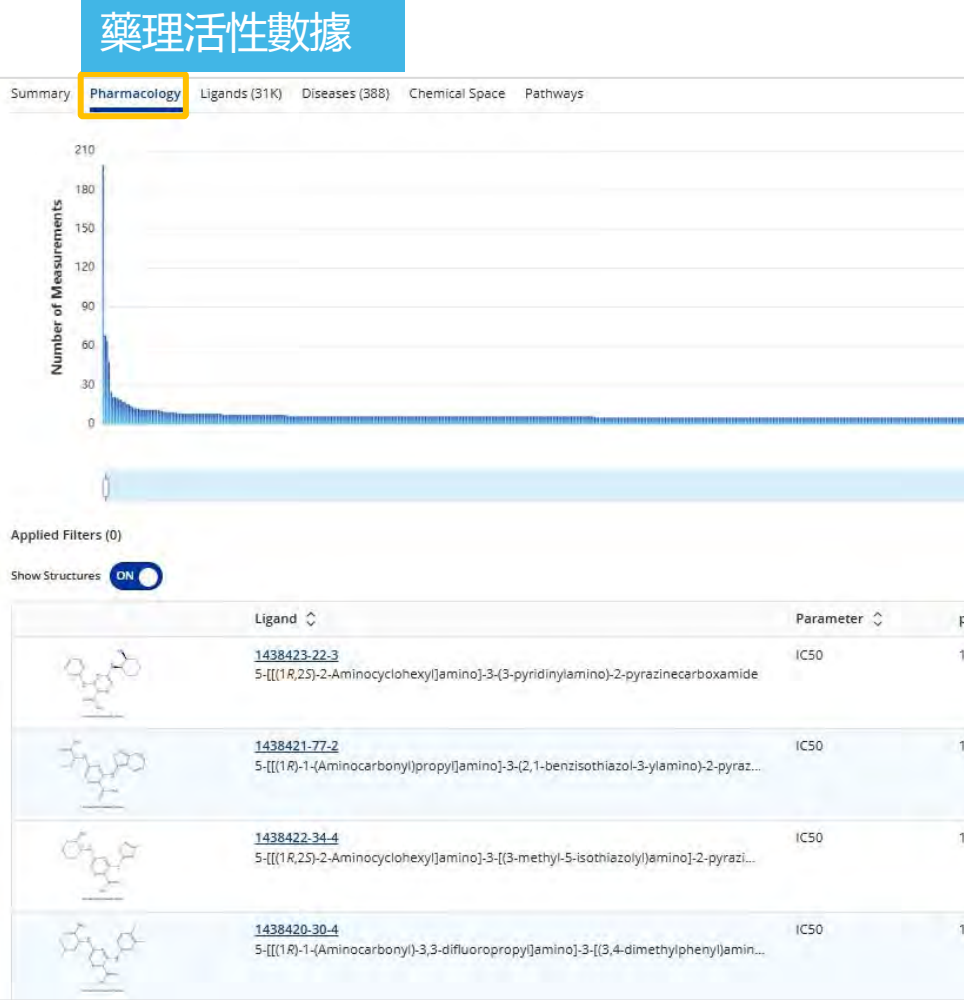
[View Less](#)

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



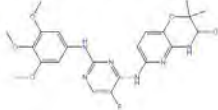
相關配體

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

Sort: Relevance

1

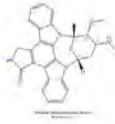
841290-80-0
6-[[[5-Fluoro-2-[(3,4,5-trimethoxyphenyl)amino]-4-pyrimidinyl]amino]-2,2-dimethyl-1,3-dioxane-5-carboxamide



Metabolites: 2 Proteins: 581

2

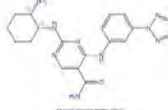
62996-74-1
Staurosporine



Metabolites: 4 Proteins: 1,024

3

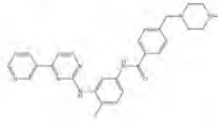
1370261-96-3
2-[[[(1R,2S)-2-Aminocyclohexyl]amino]-4-[[3-(2H-1,2,3-triazol-2-yl)phenyl]amino]-5-pyrazinecarboxamide



Metabolites: 0 Proteins: 27

4

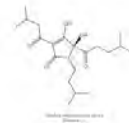
152459-95-5
Imatinib



Metabolites: 1 Proteins: 676

5

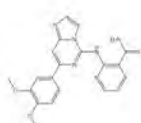
544444-90-8
(-)-cis-Tetrahydroisohumulone



Metabolites: 0 Proteins: 1

6

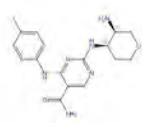
732983-37-8
2-[[[7-(3,4-Dimethoxyphenyl)imidazo[1,2-c]pyrimidin-5-yl]amino]-3-pyridinecarboxamide



Metabolites: 0 Proteins: 1

7

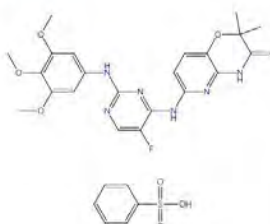
1240390-27-5
2-[[[3-(4R)-3-Amino-4-hydroxy-2H-pyran-4-yl]amino]-4-[[4-methylphenyl]amino]-5-pyrazinecarboxamide



Metabolites: 0 Proteins: 1

8

841290-81-1
Tarmatinib



Metabolites: 0 Proteins: 1

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	Reaction	Source
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}	Journal of Biological Chemistry (2001), 276(8), 5916-5923
	SLP-76 + NTP --Fibrinogen:(alpha IIb beta3)2:	Journal of Biological Chemistry (1998), 273(48), 31890-31900
	vasp + SLAP-130{p} + SLP-76{p} <=> vasp:SLAP-130{p}: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 alpha IIb beta3 initiate integrin signaling to the cytoskeleton

By: Obergfell, Adam; Eto, Koji; Mocsai, Attila; Buemacueto, Chantel; Moores, Shari 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 platelets, Src and Syk kinases are constitutively associated with alpha IIb beta3. Platelet adhesion to fibrinogen requires Src and Syk kinases. Src is localized to filopodia and cell edges. Csk, which neg. regulates Src by phosphorylation of its activation loop Tyr-529, is constitutively associated with alpha IIb beta3. Platelets multiply deficient in Src, Csk, 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 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	Database Information AN: 2002:296764 CAN: 137:106866 PubMed ID: 11940607 Cajal and MEDLINE	Company/Organization Division of Vascular Biology, Department of Cell Biology The Scripps Research Institute La Jolla, California 92037 United States	Publisher Rockefeller University Press	Language English
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一鍵連結到SciFinder文獻詳情頁

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...

0 Selected

Insulin

Hemoglobin subunit alpha 2

Hemoglobin subunit alpha 1

Hemoglobin subunit beta

Epidermal growth factor receptor

C-reactive protein

Erb-b2

Microtubule associated protein tau

Estrogen

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

Diseases search for APP

Diseases

172 Results

疾病名稱

疾病簡介

Biomarkers

生物標誌物

相關靶點與配體

Sort: Relevance

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 (Basel, 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

SummaryBiomarkersPharmacologyLigands (722K)Proteins (4,974)

Apply生物標誌物參數實驗說明有機體文獻來源

Show FiltersSummarize

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 (), 30(6), 567-76
(+)-Aldosterone	+	Pharmacodynamic/resp					
(25R)-26-Hydroxycholesterol	-	Prognostic					
[Pyruvate dehydrogenase (acetyl-transferring)] kinase isozyme 1, mitochondrial	-	Diagnostic					

(-)-Thyroxine Detail

Biomarker 51-48-9

實驗詳情

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 (), 30(6), 567-76

Health Evaluation in African Americans Using RAS Therapy

Brain Communications (2023), 5(5), 1-14

Journal of Biological Chemistry (2012), 287(44), 37245-37258

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

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, which includes fields for naming the set, selecting a color, and choosing a panel. A dropdown menu for 'Select Panel' is shown, listing various predefined sets. A text box indicates that users can 'Upload a predefined set (Optional)' by selecting a file (.sdf) or dragging and dropping it. The 'Create' button is highlighted, and a final arrow points to a context menu for the created set, which includes options like 'Rerun analysis for set', 'Add ligands from file', 'Edit set', and 'Delete set'.

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

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

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
This will automatically be applied.

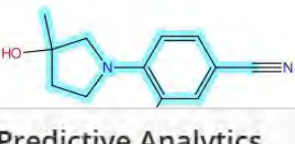
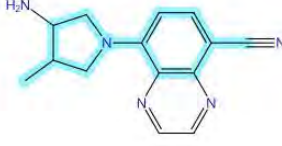
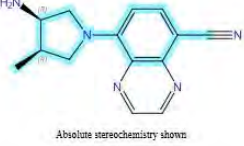
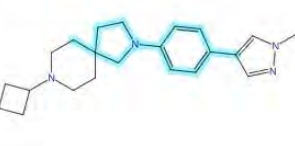
Biological Filters

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  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-quinoliny)-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

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

+ 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

Predictive_Panel_Test

Description

The full panel of protein target models available through CAS to highlight potentia

可自定义面板名称

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	A0A0S4TER9
☐ 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

Create Predictive Analytics Panel

Panel Name

Predictive_Panel_Test

Description (Optional)

Cancel

Create Panel

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)

Cancel

Save

生物活性預測結果

← [Return to Predictive Analytics](#)

Predictive_Set_09_09_2025_1002

Set Summary

Run 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](#)

▼ Organism

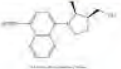
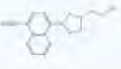
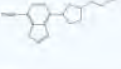
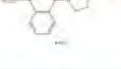
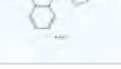
[Return to top](#)

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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