CAS BIOFINDER DISCOVERY PLATFORM™

快速使用指南 (QUICK GUIDE)

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大綱

- CAS BioFinder簡介與界面介紹
- 配體檢索與配体詳情信息（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）

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科學資訊管理對新藥研發至關重要

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洞察报告 Challenges and opportunities in data for drug discovery | CAS

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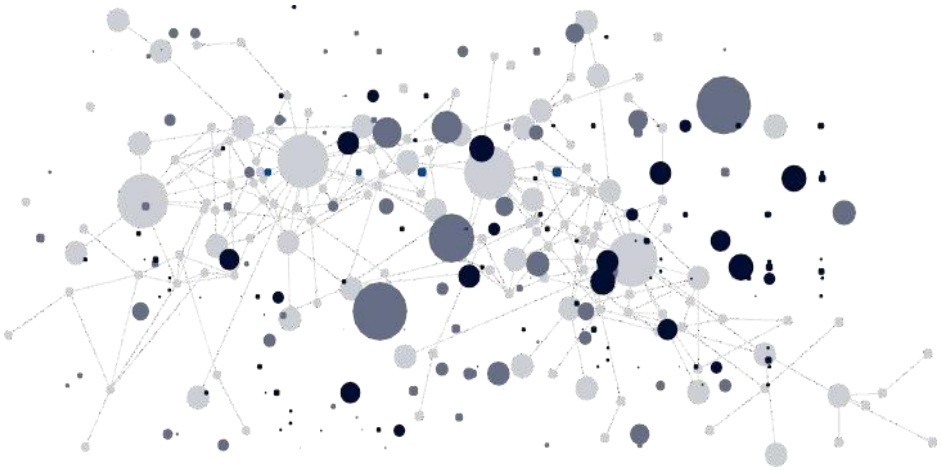
生命科學領域研究離不開重要的數據資訊基礎，但為什麼卻難以加以利用？

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

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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

耗費時間

生命科學數據量每 14 年翻一番[2]

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]。

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.

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利用CAS BioFinder 加速早期藥物研發

預測新型分子可能對生物過程產生的影響

識別與您感興趣的疾病或靶點相關的骨架和分子

發現與您感興趣的疾病相關的生物標誌物

持續開發中的更多內容與功能（序列、抗體、PDC、藥物情報等）

找出哪些候選藥物最有可能成為最安全、最佳的先導化合物

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CAS BioFinder檢索介面

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- CAS BioFinder簡介與檢界面介紹（介紹與介面）
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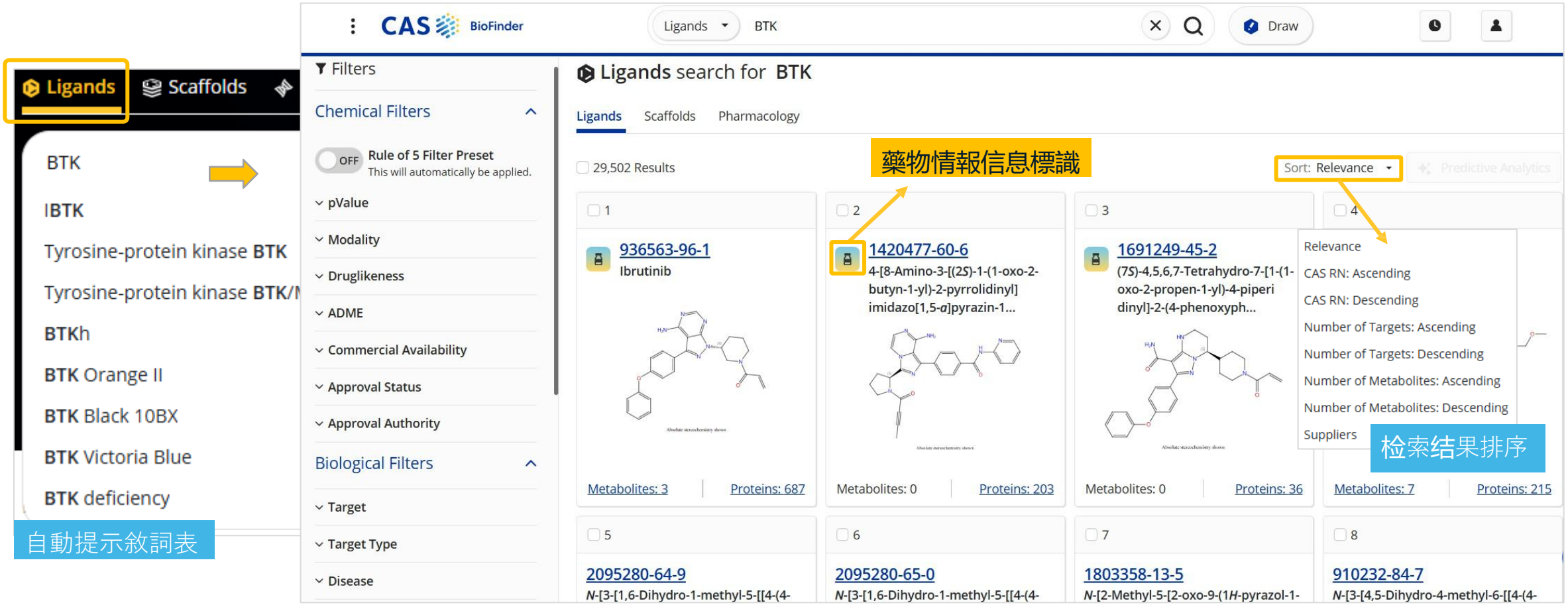
基於靶點、疾病、藥物名稱以及結構，檢索資訊



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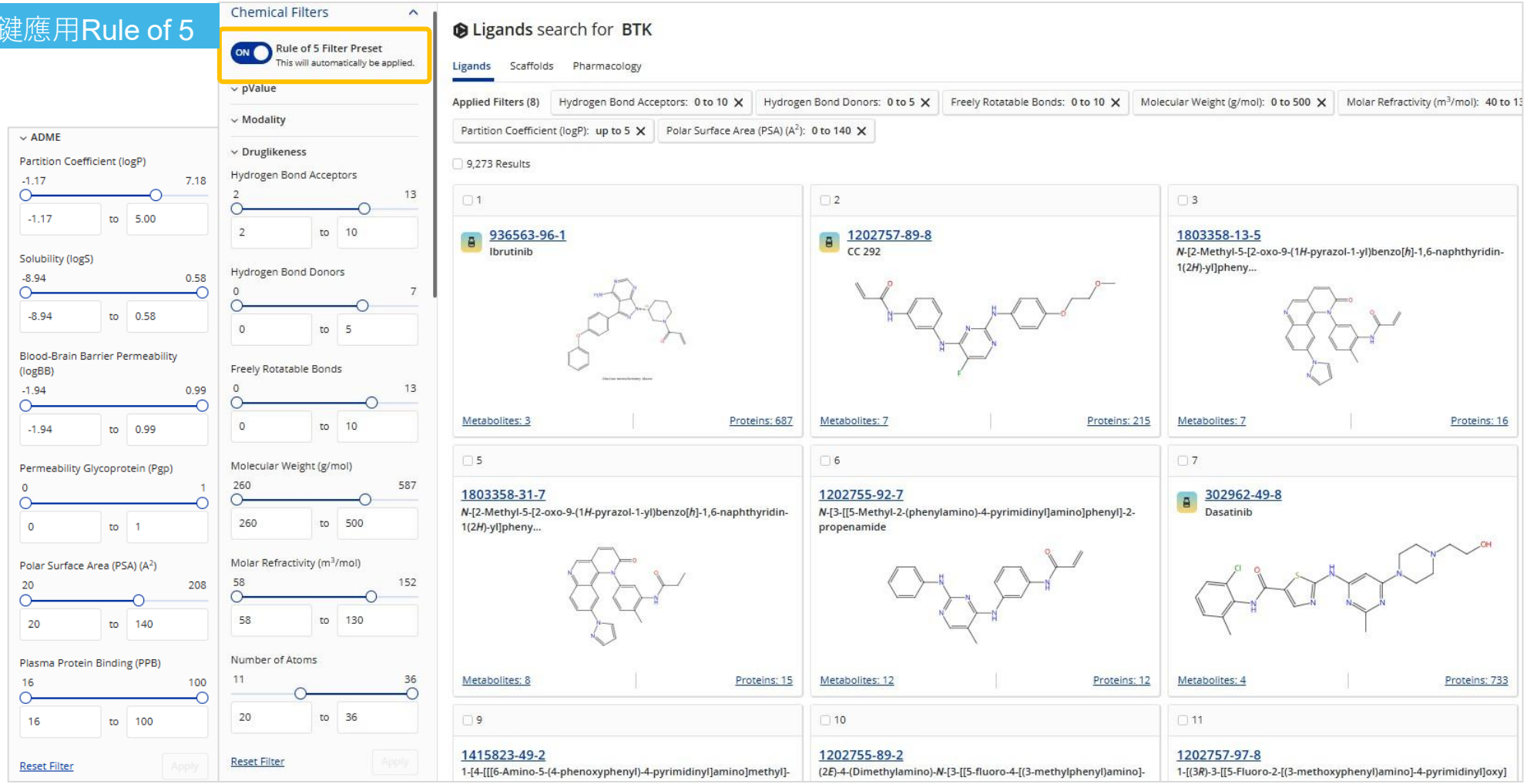
篩選具有類似先導化合物特性的小分子配體

一鍵應用Rule of 5



- 氫键受體<10
- 氫键供體<5
- 自由旋轉键 <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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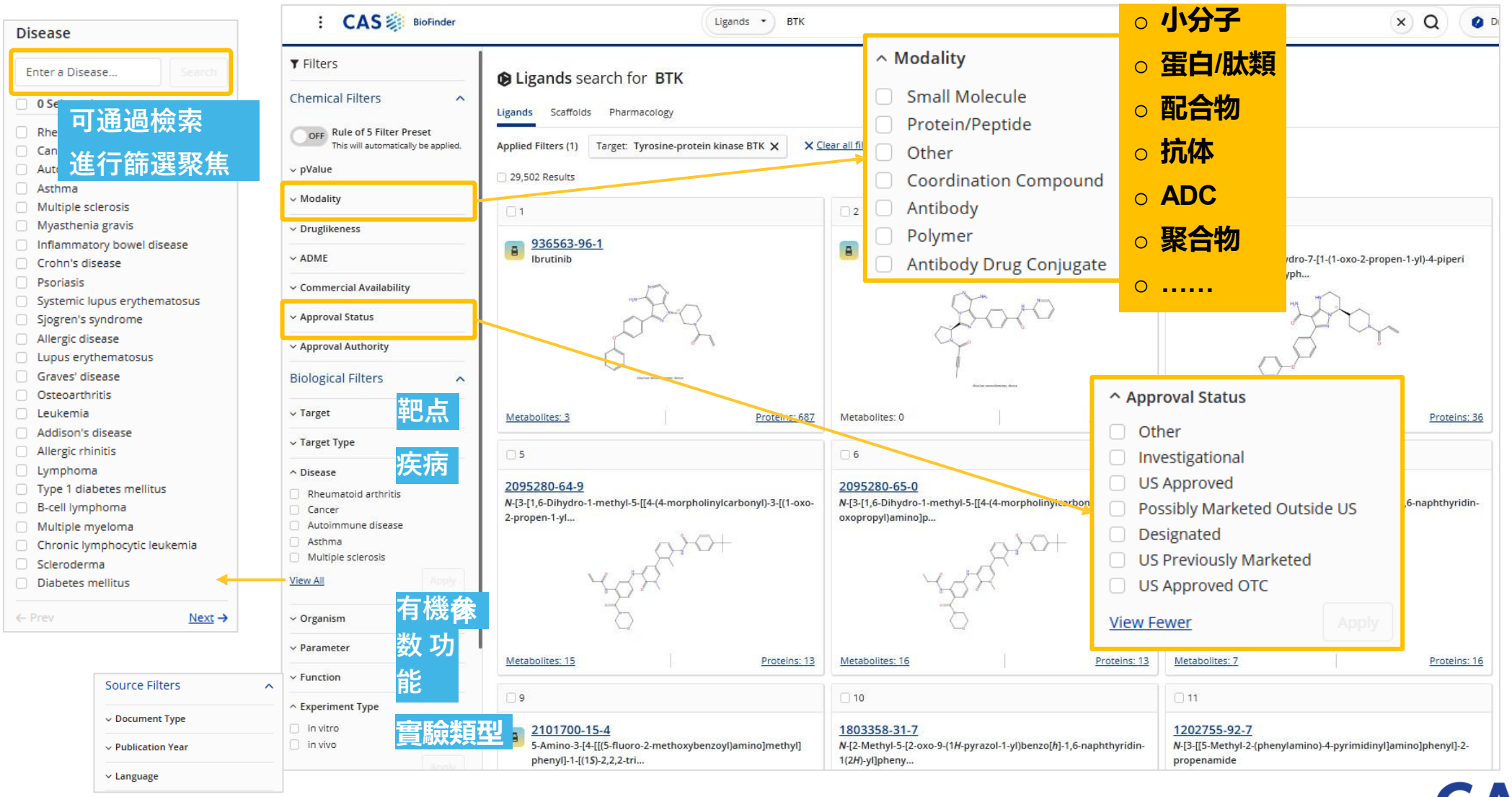
配體檢索結果的縱覽與聚焦



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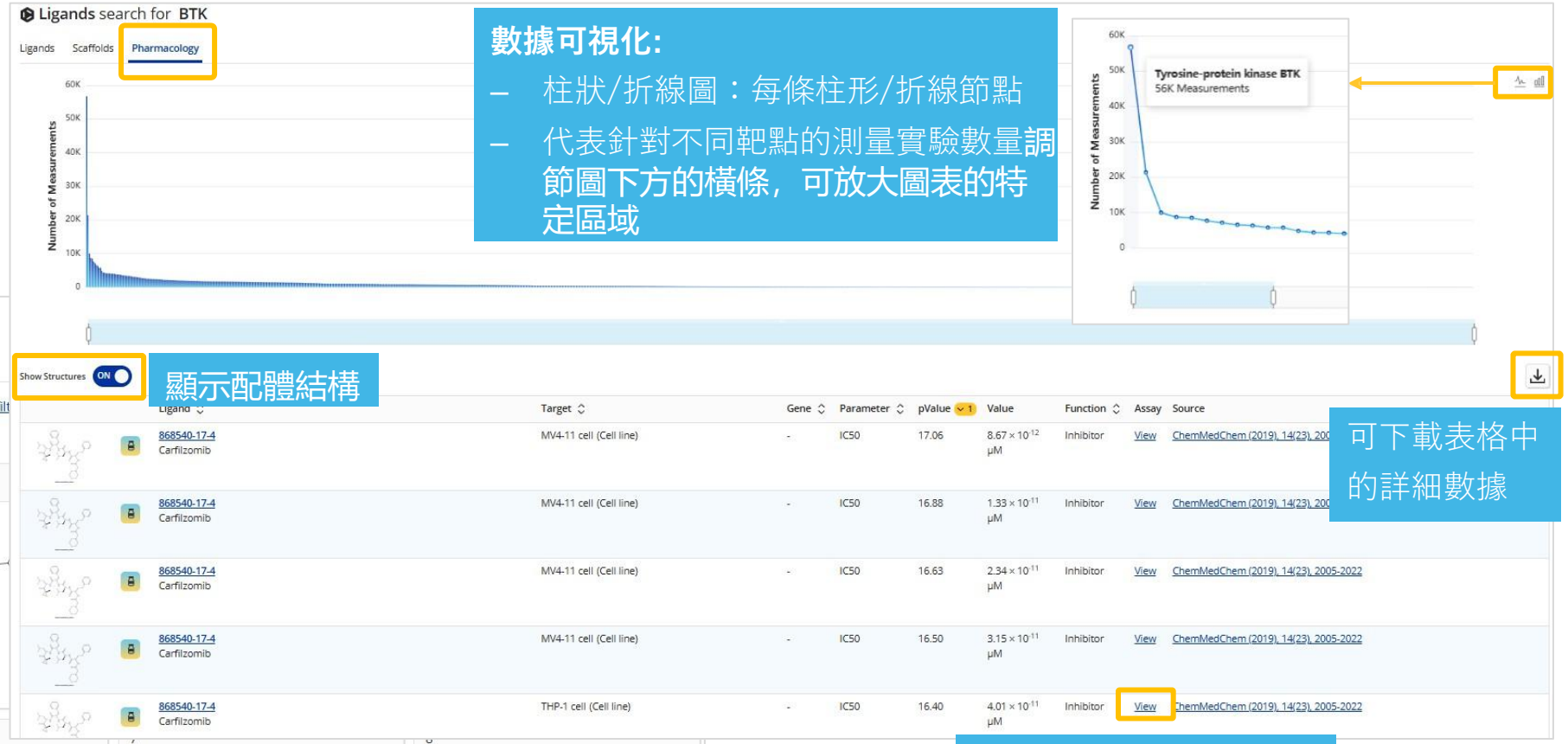
縱覽配體檢索結果集相關骨架結構與藥理學數據

查看配體檢索結果關聯的骨架結構



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

顯示配體結構

可下載表格中的詳細數據

點擊View，可查看原文中的Assay的細節

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探索配體的詳細資訊

Doxorubicin
CAS Registry Number: 23214-92-8

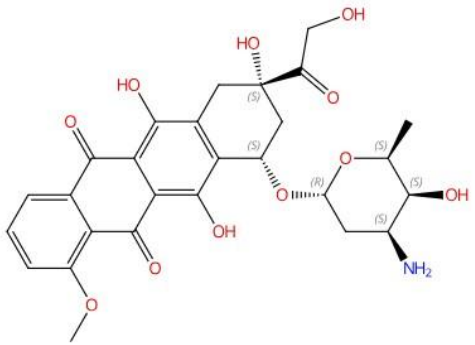
112K | 1,642 | Retrosynthesis | Predictive Analytics | ...

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)

配體相關信息標籤頁



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-, (8*S*,10*S*)-

藥物情報資訊

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 View All
PRIMARY TARGET	DNA topoisomerase II **Function:** Inhibitor **Measurement:** IC50 2.67 μM Source View All

View Related Drugs

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)

Canonical SMILES
O=C1C=2C=CC=C(OC)C2C(=O)C=3C(O)=C4C(=C(O)C13)CC(O)(C(=O)CO)CC4OC5OC(C)C(O)C(N)C5

Isomeric SMILES
OC=1C2=C([C@@H](O[C@H]3C[C@H](N)[C@H](O)[C@H](C)O3)C[C@@](C(CO)=O)(O)C2)C(O)=C4C1C(=O)C=5C(C4=O)=C(OC)C=CC5

InChI
InChI=1S/C27H29NO11/c1-10-22(31)13(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
AOJJSUZBOXZQNB-TZSSRYMLSA-N

22 other names for this Ligand
- (7S,9S)-7-[(2R,4S,5S,6S)-4-Amino-5-hydroxy-6-methyloxan-2-yl]oxy-6,9,1 1-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)-

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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

STATUS

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

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

View Related Drugs

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

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 carcino			View
Pancreatic ductal adenocar			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. Medications/emergency equipment to treat such reactions should be available for immediate use (5.2).**
- **Severe myelosuppression may occur (5.3)**
- **Reduce dosage in patients with impaired hepatic function (2.6).**
- **Accidental substitution of DOXIL resulted in severe side effects. Do not substitute on mg per mg basis with doxorubicin HCl (2.1).**

----------**RECENT MAJOR CHANGES**----------
Contraindications, Nursing Mothers (4) Removed 9/2012
Warnings and Precautions, Secondary Oral Neoplasms (5.9) 8/2013

----------**INDICATIONS AND USAGE**----------
DOXIL is an anthracycline topoisomerase inhibitor indicated for:
- **Ovarian cancer (1.1)**
After failure of platinum-based chemotherapy.
- **AIDS-related Kaposi's Sarcoma (1.2)**
After failure of prior systemic chemotherapy or intolerance to such therapy.
- **Multiple Myeloma (1.3)**
In combination with bortezomib in patients who have not previously received bortezomib and have received at least one prior therapy.

----------**DOSAGE AND ADMINISTRATION**----------
Administer DOXIL at an initial rate of 1 mg/min to minimize the risk of infusion reactions. If no infusion related reactions occur, increase rate of infusion to complete administration over 1 hour. Do not administer as bolus injection or undiluted solution (2.1).
- **Ovarian cancer:** 50 mg/m² IV every 4 weeks for 4 courses minimum (2.2)
- **AIDS-related Kaposi's Sarcoma:** 20 mg/m² IV every 3 weeks (2.3)
- **Multiple Myeloma:** 30 mg/m² IV on day 4 following bortezomib which is administered at 1.3 mg/m² bolus on days 1, 4, 8 and 11, every 3 weeks (2.4)

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

----------**CONTRAINDICATIONS**----------
- Hypersensitivity reactions to a conventional formulation of doxorubicin HCl or the components of DOXIL (4, 5.2)

----------**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 (1-800-526-7736) 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

FULL PRESCRIBING INFORMATION: CONTENTS*

WARNING– INFUSION REACTIONS, MYELOSUPPRESSION, CARDIOTOXICITY, LIVER IMPAIRMENT, ACCIDENTAL SUBSTITUTION
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1.2 AIDS-Related Kaposi's Sarcoma
1.3 Multiple Myeloma
2 DOSAGE AND ADMINISTRATION
2.1 Usage and Administration Precautions
2.2 Patients With Ovarian Cancer
2.3 Patients With AIDS-Related Kaposi's Sarcoma
2.4 Patients With Multiple Myeloma
6 ADVERSE REACTIONS
6.1 Overall Adverse Reactions Profile
6.2 Adverse Reactions in Clinical Trials
6.3 Post Marketing Experience
7 DRUG INTERACTIONS
8 USE IN SPECIFIC POPULATIONS
8.1 Pregnancy
8.3 Nursing Mothers
8.4 Pediatric Use
8.5 Geriatric Use
8.6 Hepatic Impairment
10 OVERDOSAGE
11 DESCRIPTION
12 CLINICAL PHARMACOLOGY

FDA文件的pdf

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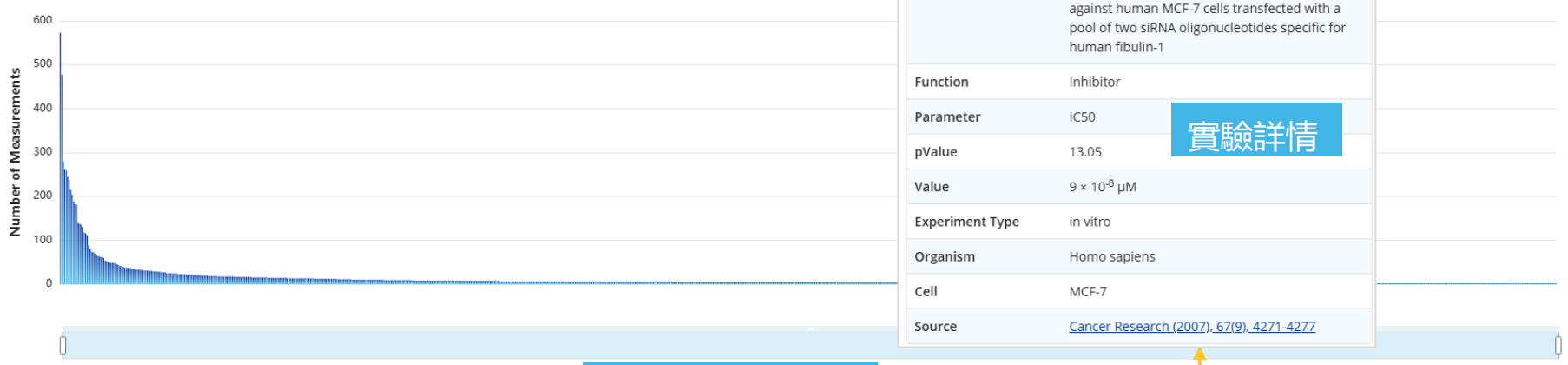
配體藥理學資訊

Summary | Pharmacology | ADME | Toxicology | Proteins (313) | Diseases (301) | Related Immunotherapeutics (12) | Chemical Space | Metabolite



← 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	9×10^{-8} μM
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

Applied Filters (0)

可自定義排序方式

Show Filters

Target	Gene	Parameter	pValue 1	Value	Function	Organism	Assay	Source
Fibulin-1 (Protein)	FBLN1	IC50	13.05	9×10^{-8} μM	Inhibitor	Homo sapiens	View	Cancer Research (2007), 67(9), 4271-4277
Fibulin-1 (Protein)	FBLN1	IC50	12.10	8×10^{-7} μM	Inhibitor	Homo sapiens	View	Cancer Research (2007), 67(9), 4271-4277
Fibulin-1 (Protein)	FBLN1	IC50	12.00	1×10^{-6} μM	Inhibitor	Homo sapiens	View	Cancer Research (2007), 67(9), 4271-4277
Fibulin-1 (Protein)	FBLN1	IC50	12.00	1×10^{-6} μM	Inhibitor	Homo sapiens	View	Cancer Research (2007), 67(9), 4271-4277
K562 (Cell line)	-	IC50	11.30	5×10^{-6} μM	-	Homo sapiens	View	Biochemical Pharmacology (2004), 68(10), 1911-1922
MDA-MB-231 (Cell line)	-	IC50	10.33	4.7×10^{-5} μM	-	Homo sapiens	View	Journal of Medicinal Chemistry (2011), 54(1), 411-415

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 | Apply

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

View All | Apply

Function
- Inhibitor
- Modulator
- Binder
- Substrate
- Antagonist

View All | Apply

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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
0.918	-3.27	-1.96	206.07	67.32	1

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

Applied Filters (0)

Show Filters

Parameter ^1	Value	Organism	Assay	Sou	
t1/2	9.63 hr	Rattus	View	Inte	, Netherlands) (2019), 557(), 264-272
t1/2	32 hr	Rattus	View	Jou	
t1/2	6.8 hr	Macaca mulatta	View	Ant	4), 1100-1101
t1/2	5.7 hr	Mus	View	Adv	2(50), 2004385
t1/2	11.9 hr	Mus musculus	View	Wo	06824 A1 2013-07-18
t1/2	17.9 hr	Rattus	View	Inte	2023), 228(), 273-285
t1/2	3.5 hr		View	Bio	
t1/2	0.8 hr		View	AAF	
t1/2	15.9 hr		View	Ana	2), 4279-4288
Vd	970.8667 L/		View	Inte	, Netherlands) (2017), 526(1-2), 443-454

← 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

Filters

Biological Filters

Organism

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

View All Apply

生物有機體

Parameter

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

View All Apply

代謝相關參數

Experiment Type

- in vivo
- in vitro

Apply

實驗類型

Source Filters

- Document Type
- Publication Year
- Language

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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 1	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/yea
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/yea
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)/pag
IC50	4.8 mg/L	Mus musculus	View	JOET ck, Ireland) V.1- 1979- Volume(issue)/page/yea

← 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

Biological Filters 毒理學實驗數據篩選項

Show Filters

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

View All

生物有機 體

Parameter
- LC50
- IC50
- LD50
- MTD
- LDLo

View All Apply

毒理學參數

Experiment Type
- in vitro
- in vivo

Apply

實驗類型

Route of Administration
- Intraperitoneal
- Intravenous
- Oral
- Immersion
- Subcutaneous

Apply

給藥方式

Source Filters

Document Type

Publication Year

Language

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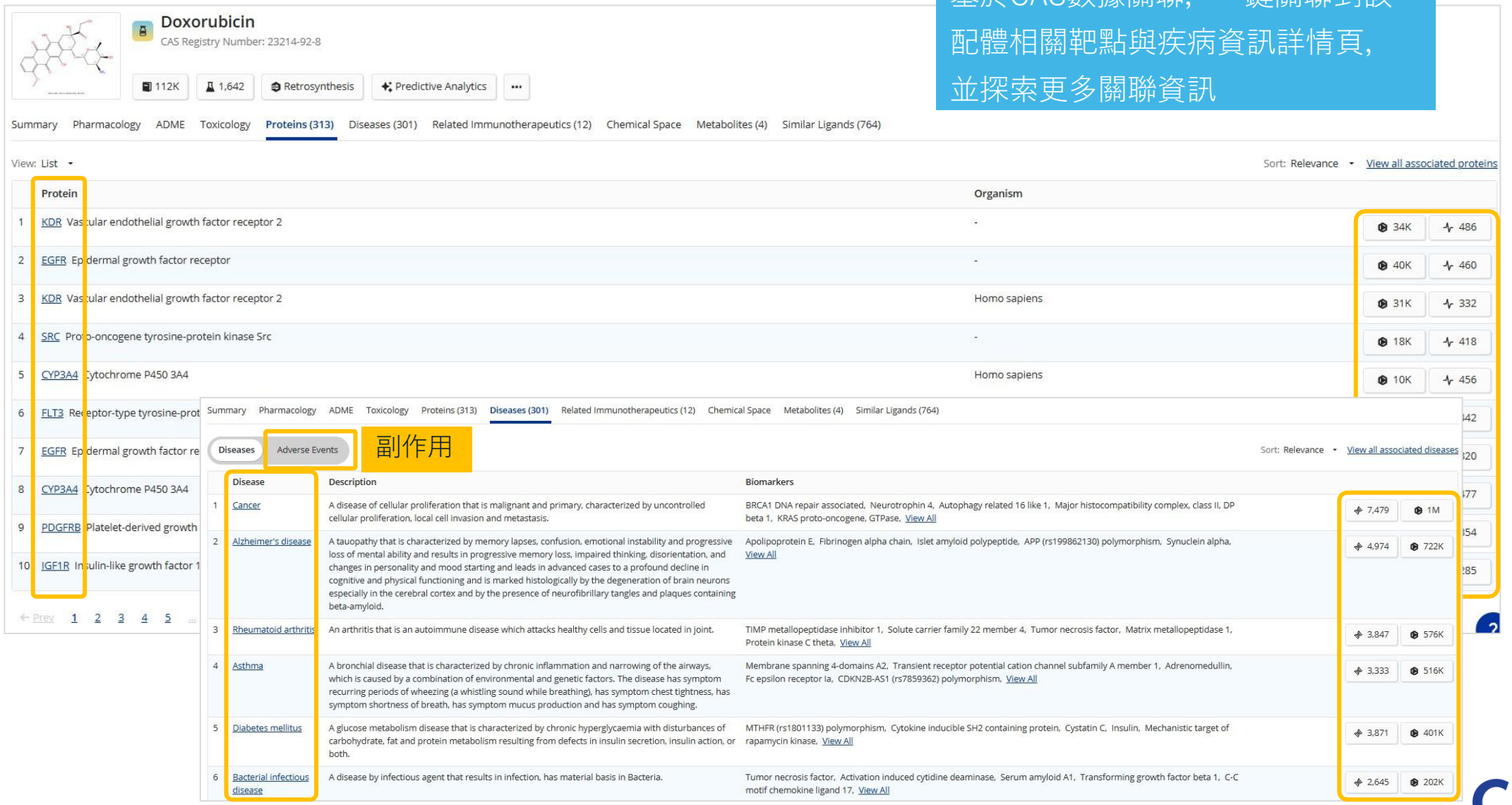
配體相關靶點與疾病資訊

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



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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)

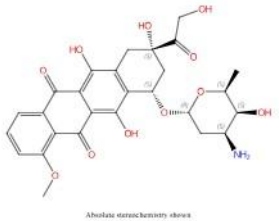
MAb-DMBA-SIL-Dox

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.

免疫療法詳情

抗體與配體結構資訊

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.

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ADC藥物詳情

Trastuzumab emtansine

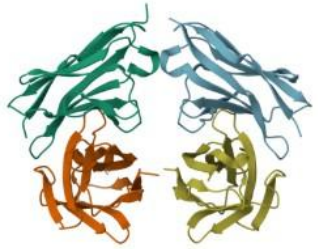
CAS Registry Number: 1018448-65-1

1,972 | 8 | Retrosynthesis | Predictive Analytics | ...

Summary | Pharmacology | ADME | Proteins (2) | Diseases (1)

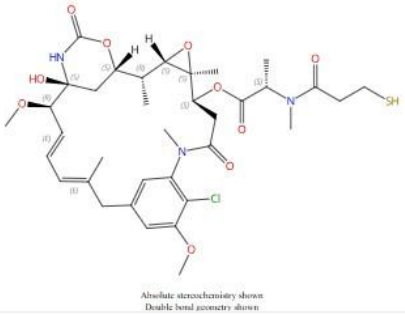
Antibody	Trastuzumab
Antigen	Receptor tyrosine-protein kinase erbB-2 (ERBB2)
Payload	Mertansine DM1
Therapeutic Target	Microtubule
Drug-Antibody Ratio	3.5
Linker	Succinimidyl-4-(N-maleimidomethyl)cyclohexane-1-carboxylate (SMCC)
Method	Random conjugation through nucleophilic lysines.

ADC藥物詳情



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

EVQLVESGGGLVQPGGSLRLSCAASGGFNIKDTYIHWVRQAPGKGLEWVARIYPTNGYTTRYADSVKGRFTISADTSKNTAYLQMNSLRAEDTAVYYSRWGGDG
FYAMDYDYWGQGTLVTVSSASTKGPSVFPLAPSSKSTSGGTAALGCLVKDYFPEPVTVSWNSGALTSGVHTFPAVLQSSGLYSLSSVVTVPSSSLGTQTYICNV
NHKPSNTKVDKKVEPKSCDKTHTCPPCPAPELLGGPSVFLFPPKPKDTLMISRTPEVTCVVVDVSHEDPEVKFNWYVDGVEVHNAKTKPREEQYNSTYRVVSVL
TVLHQDWLNGKEYKCKVSNKALPAPIEKTISKAKGQPREPQVYTLPPSREEMTKNQVSLTCLVKGFYPSDIAVEWESNGQPENNYKTTPPVLDSDGSFFLYSKL
TVDKSRWQQGNVFSCSVMHEALHNHYTQKSLSLSPGK

重鏈/輕鏈序列

Light Chain Sequence

DIQMTQSPSSLSSASVGDRVTITCRASQDVNTAAVAWYQQKPGKAPKLLIYSASFLYSGVPSRFSGSRSGTDFTLTISSLQPEDFATYYQQHYTTPPTPTFGQG
TKVEIKRTVAAPSVFIFPPSDEQLKSGTASVVCLLNNFYPREAKVQWKVDNALQSGNSQESVTEQDSKDSTYSLSSTLTLSKADYEKHKVYACEVTHQGLSSPV
TKSFNRGEC

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

CDR序列

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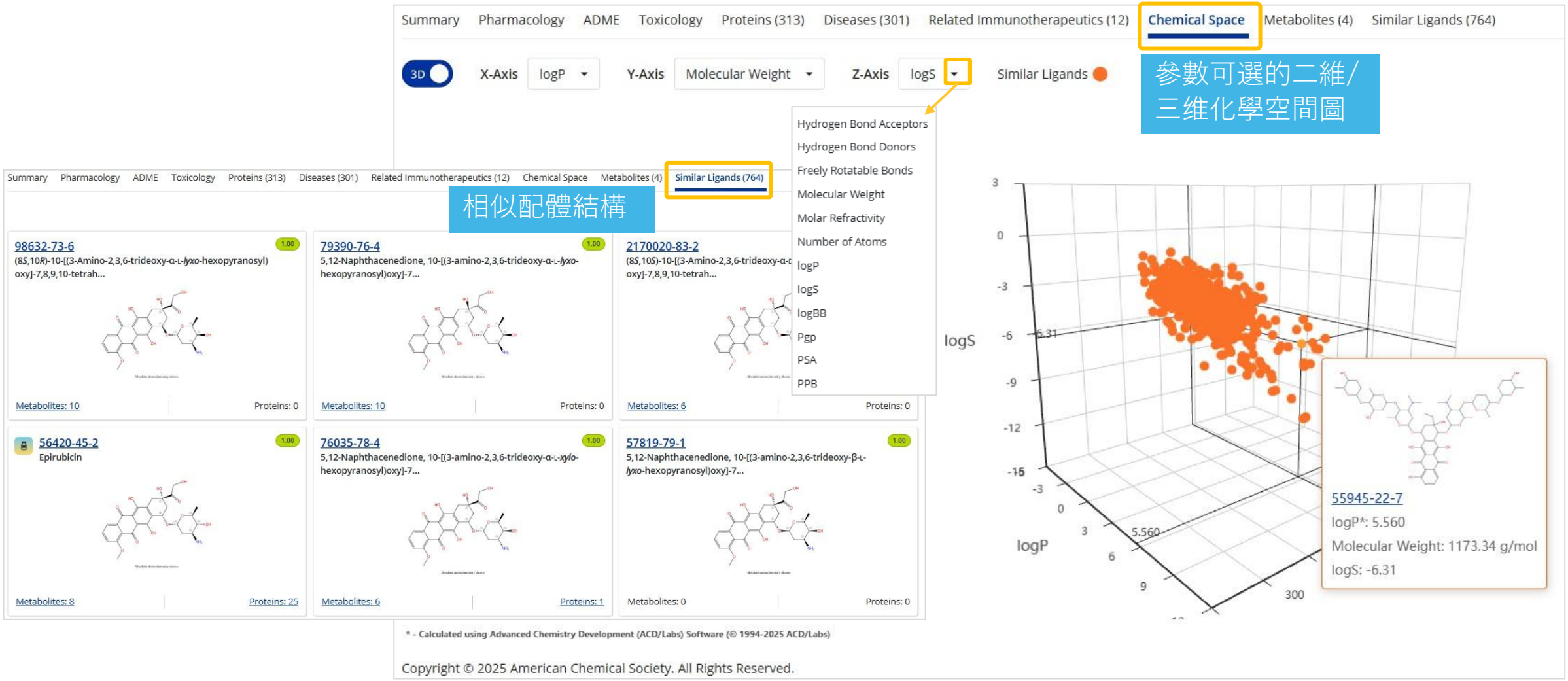
相似配體結構與可視化分析



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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

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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 ）

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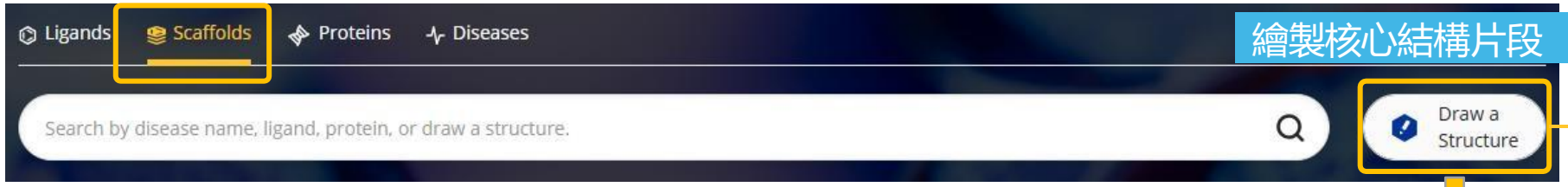
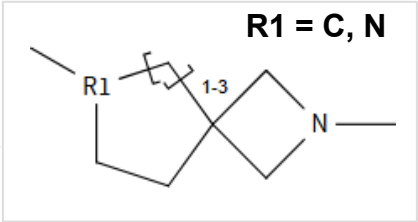
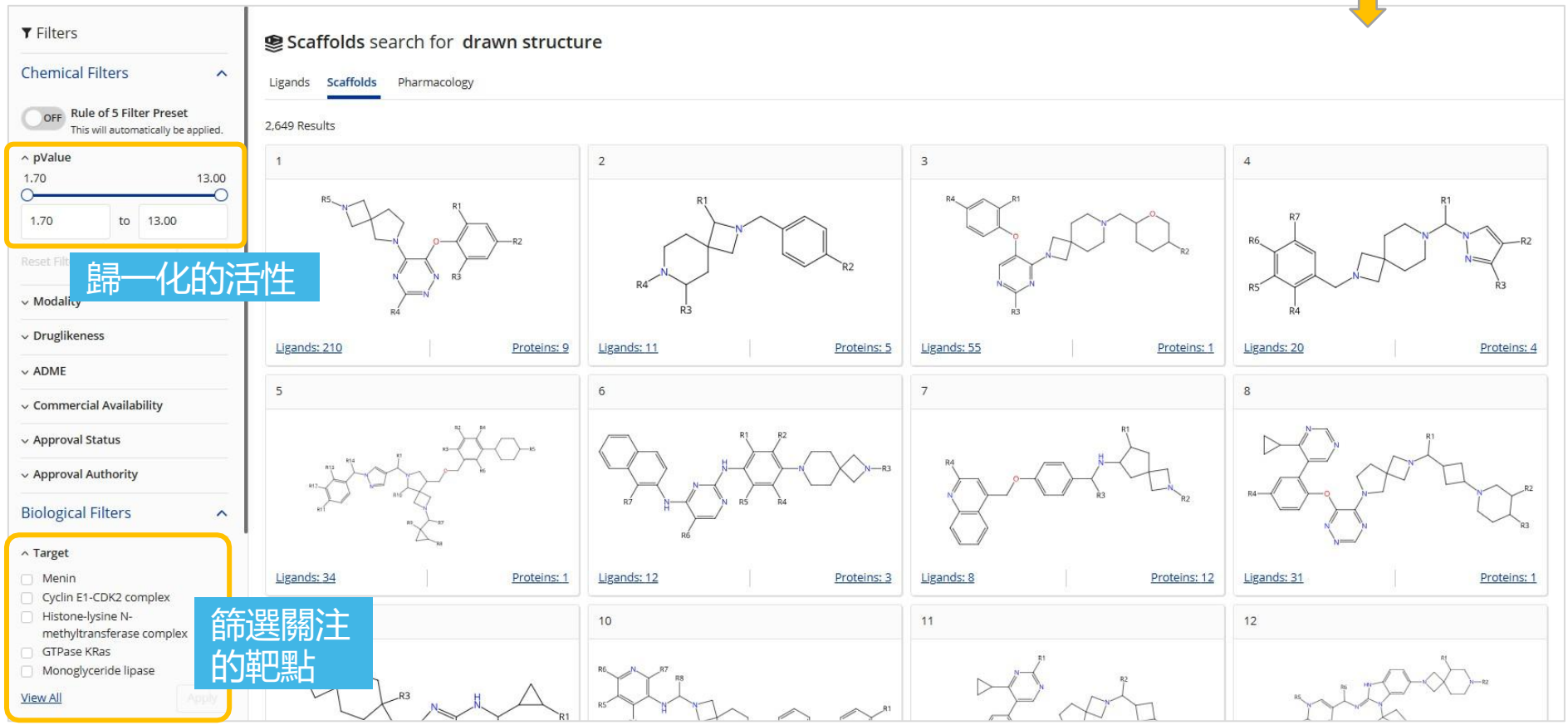
基於靶點或結構片段，探索活性結構骨架







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

IC50越小，pValue越大，抑制活性越高。

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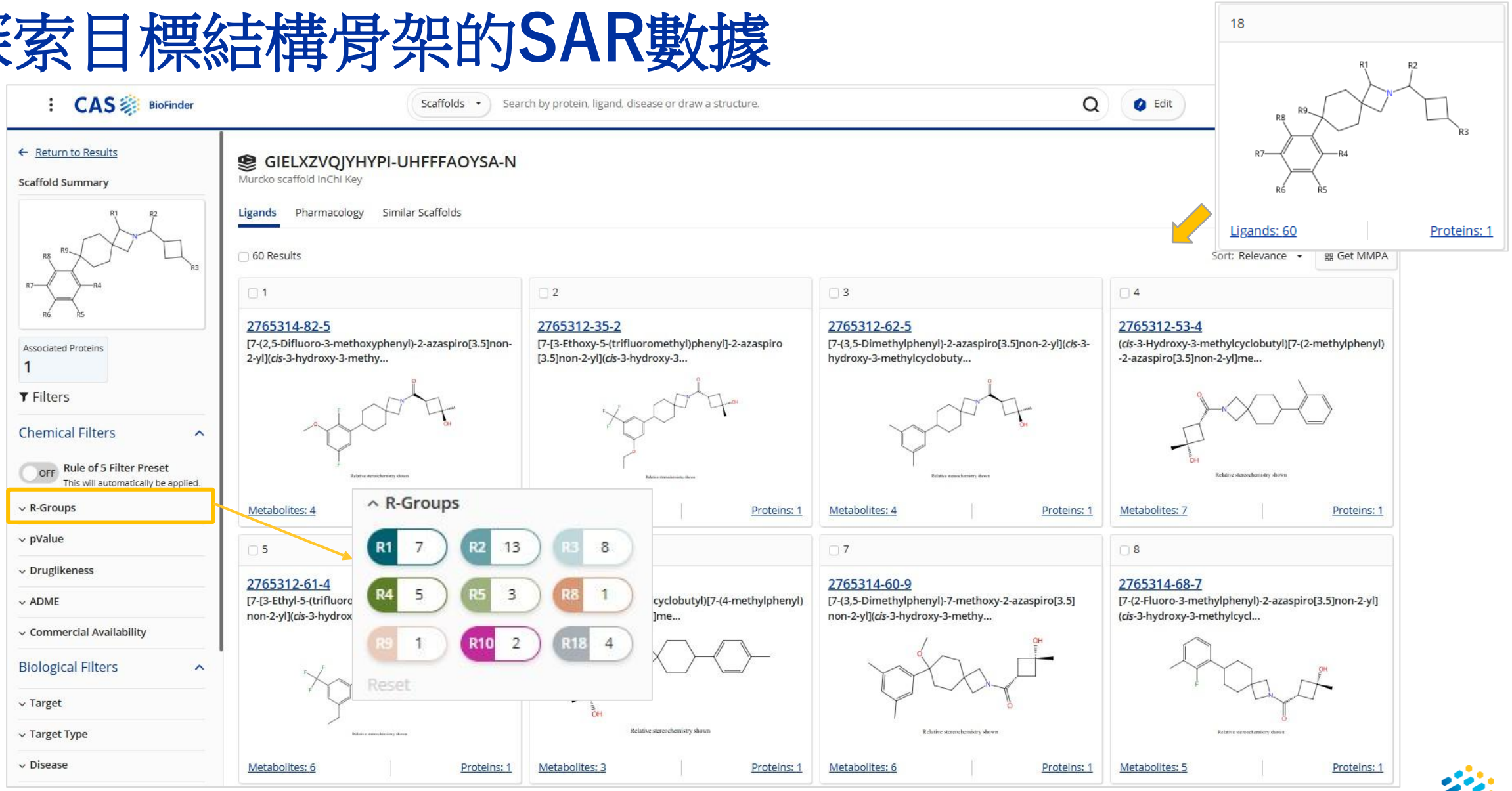
探索目標結構骨架的SAR數據



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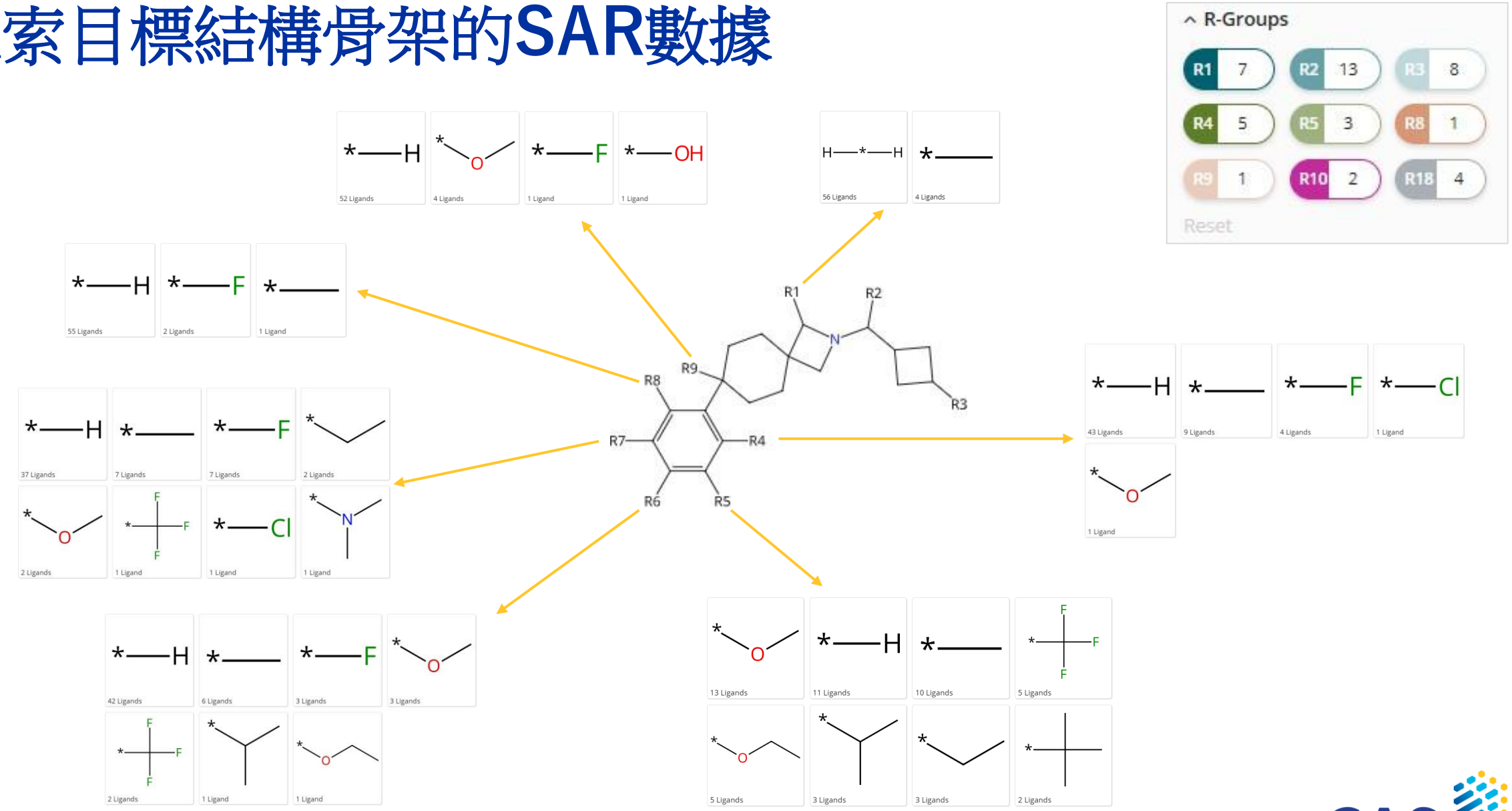
探索目標結構骨架的SAR數據



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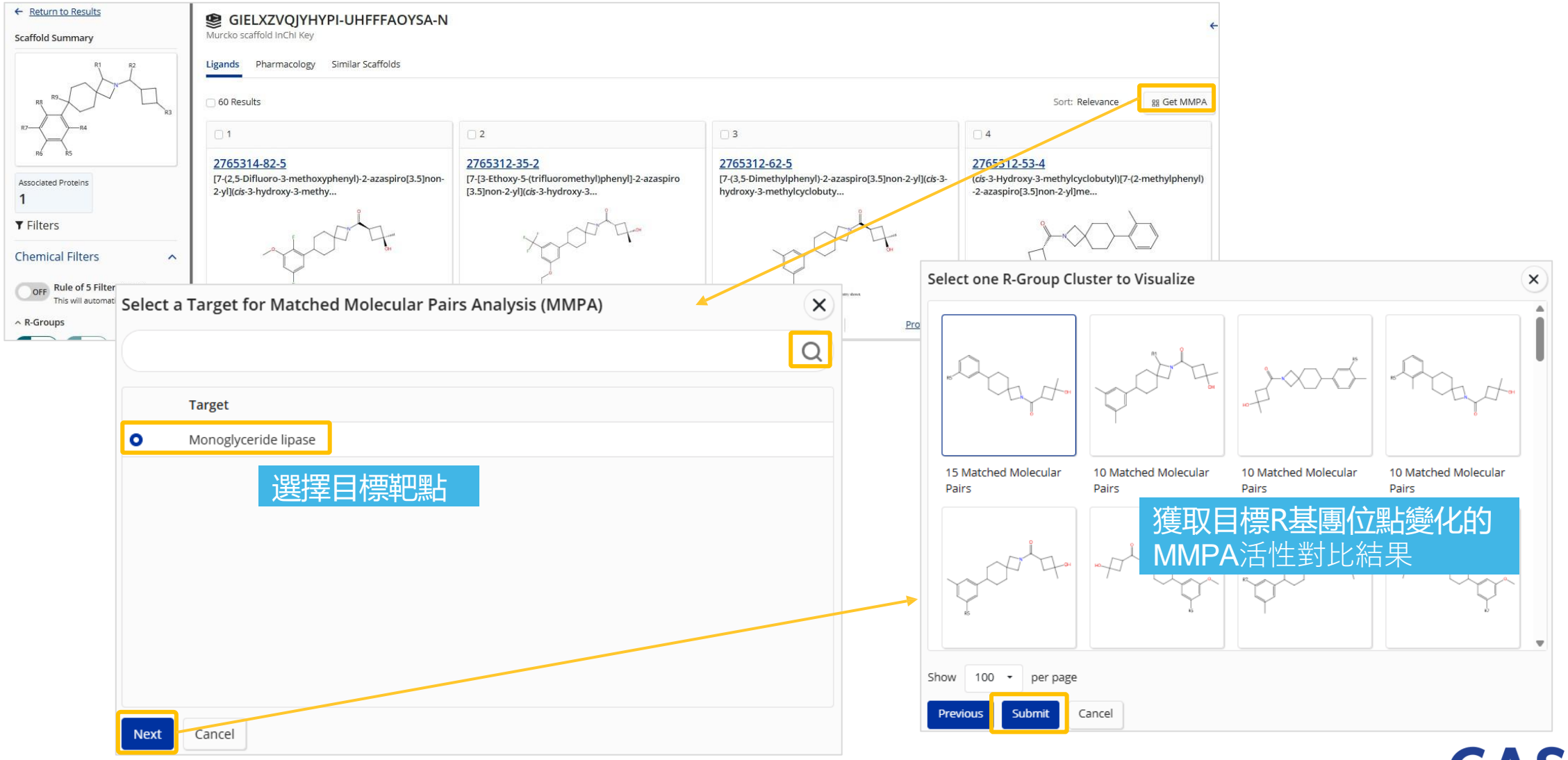
符合分子對分析（MMPA）



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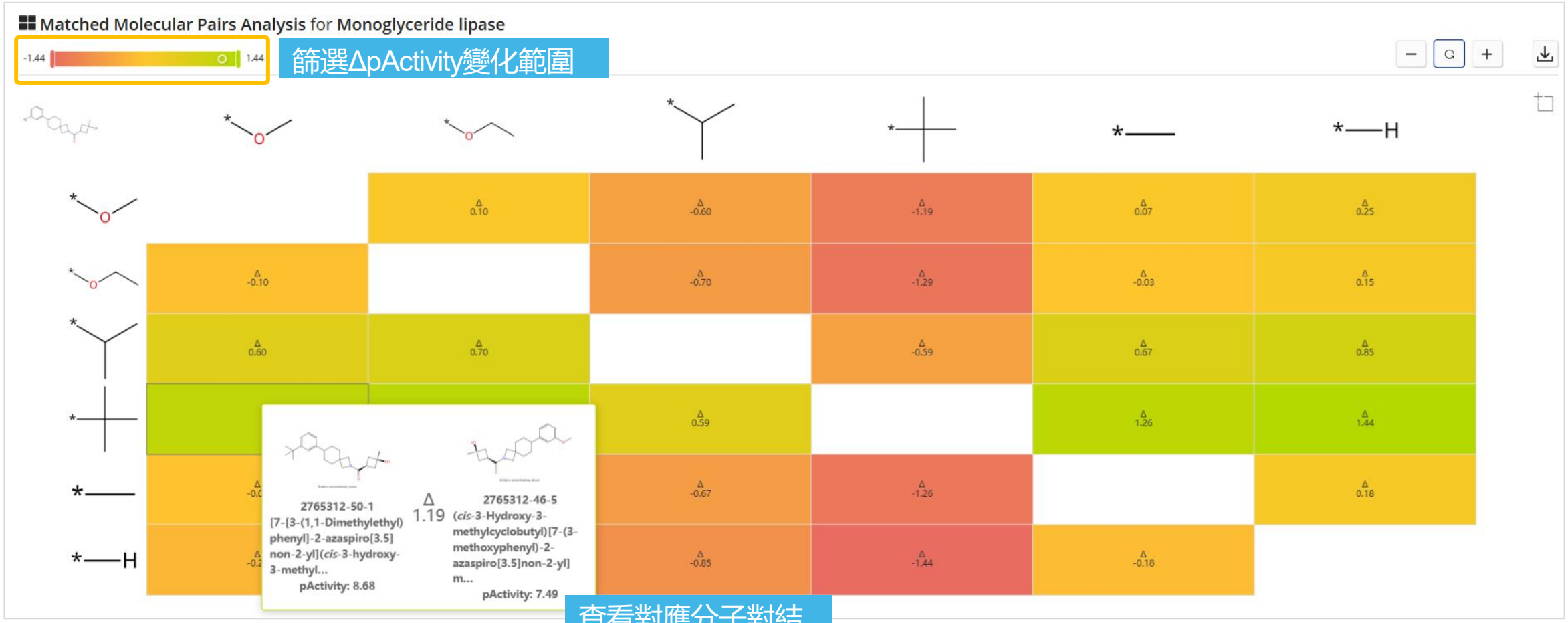
符合分子對分析（MMPA）

快速直觀獲取匹配分子對ΔpActivity熱圖



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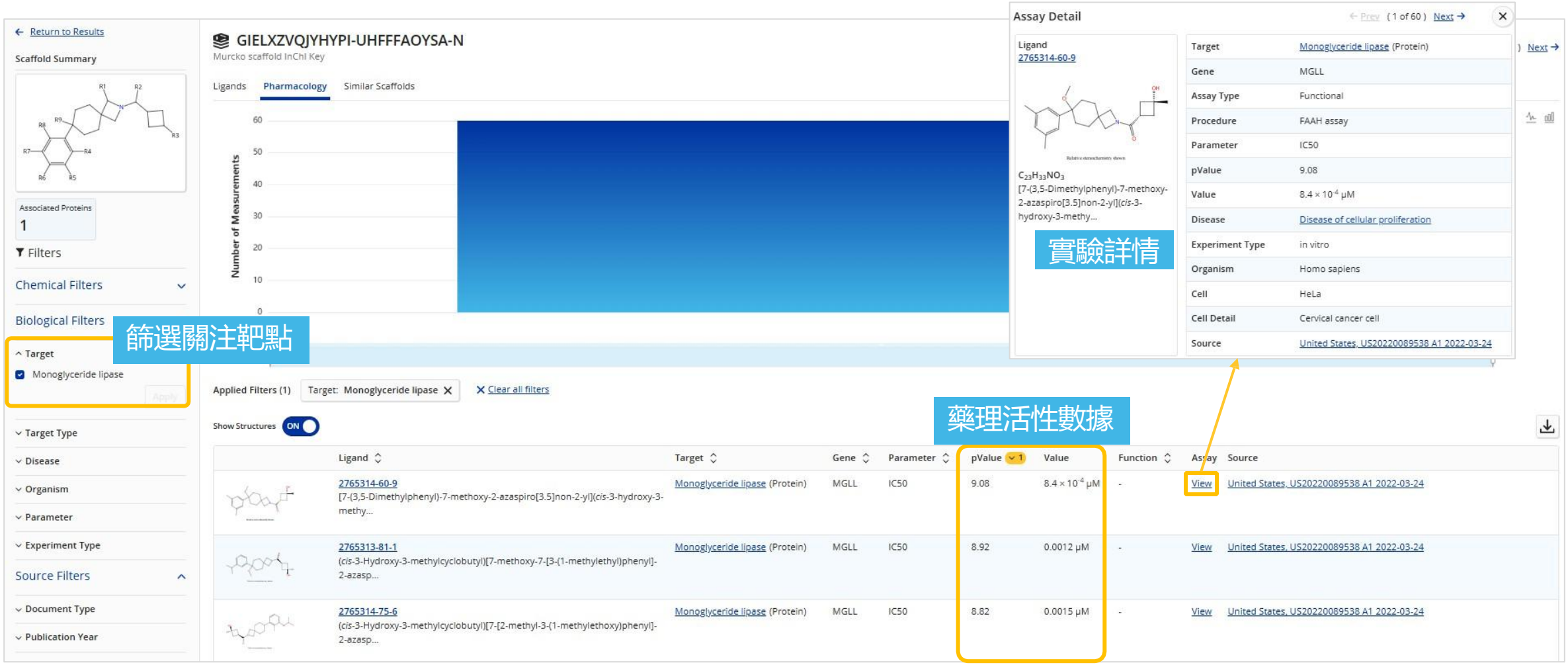
查看同一結構骨架中的配體藥理活性



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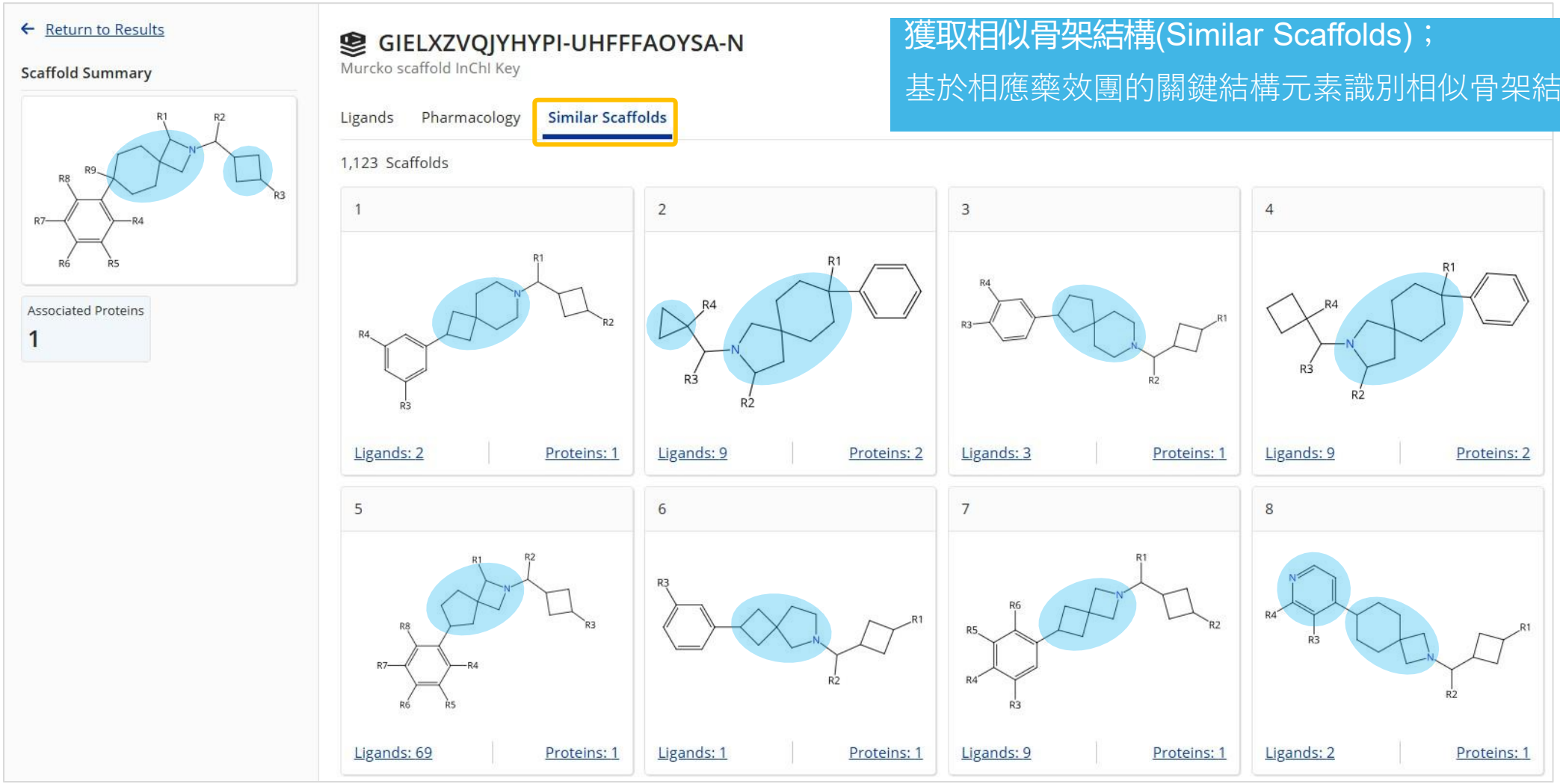
獲取與目標骨架相似骨架結構，啟發新的SAR假設

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



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- 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）

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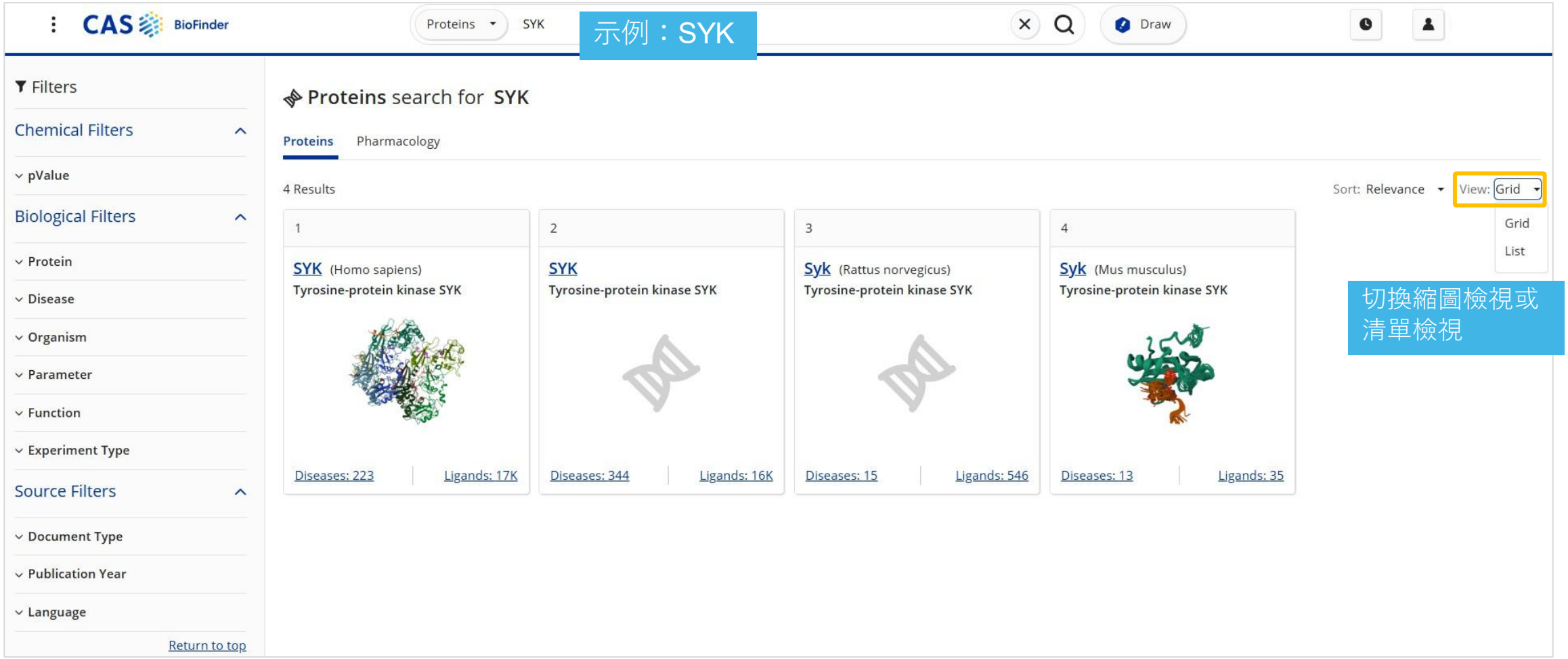
通過靶點、疾病或配體，獲取歸一化的蛋白檢索結果



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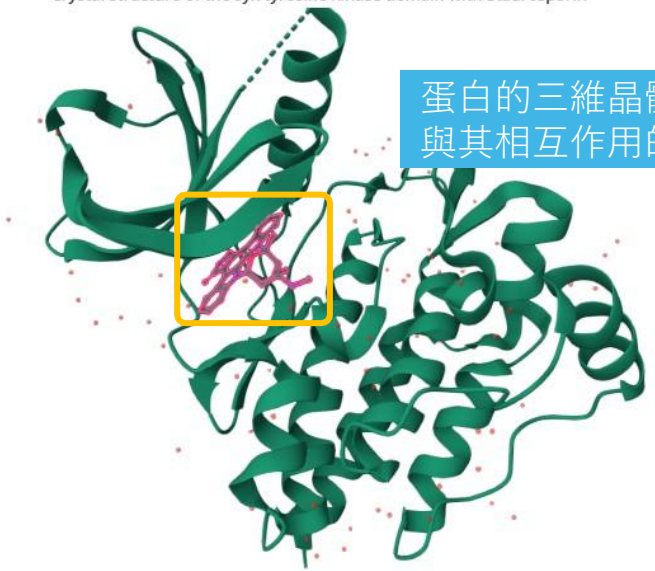
蛋白詳情資訊與立體結構展示

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

STAUROSPORINE
1XBC | Model 1 | Instance ASM_1 | B [auth A] | STU 1

1XBC 下載cif格式結構檔

Organism

Homo sapiens
unspecified
Rattus norvegicus
Mus musculus

來源有機體

Homo sapiens | GET FASTA | Copy Sequence

```
>P43405-1|Tyrosine-protein kinase SYK|Homo sapiens
MASSGMADSANHLPFFFGNITREEAEDYLVQGGMSDGLYLLRQSRNYLGGFALSVAHGRKAHHYTIERELNGTYAIAGGRTHASPADLCHYHSQESDGLVCLLKKPFNRPQGVQPK
TGPFEDLKENLIREYVKQTWNLQGQALEQAIISQKPQLEKLIATTAHEKMPWFHGKISREESEQIVLIGSKTNGKFLIRARDNNGSYALCLLHEGKVLHYRIDKDKTGKLSIPEGK
KFDTLWQLVEHYSYKADGLLRVLTVPCQKIGTQGNVNFGGRPQLPGSHPATWSAGGIISRIKSYSFPKPGHRKSSPAQGNRQESTVSFNPYEPELAPWAADKGPQREALPMDTEVY
ESPYADPEEIRPKEVYLDRKLLTLEDKELGSGNFGTVKKGYYQMKKVVKTVAVKILKNEANDPALKDELLAEANVMQQLDNPYIVRMIGICEAESWMLVMEMAELGPLNKYLQQNR
HVKDKNIIELVHQVSMGMKYLEESNFVHRDLAARNVLLVTQHYAKISDFGLSKALRADENYYKAQTHGKWPVKWYAPECINYYKFSSKSDVWSFGVLMWEAFSYGQKPYRGMKGSE
VTAMLEKGERMGCPAGCPREMYDLMNLCWTYDVENRPGFAAVELRLRNYYYDVVN
```

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

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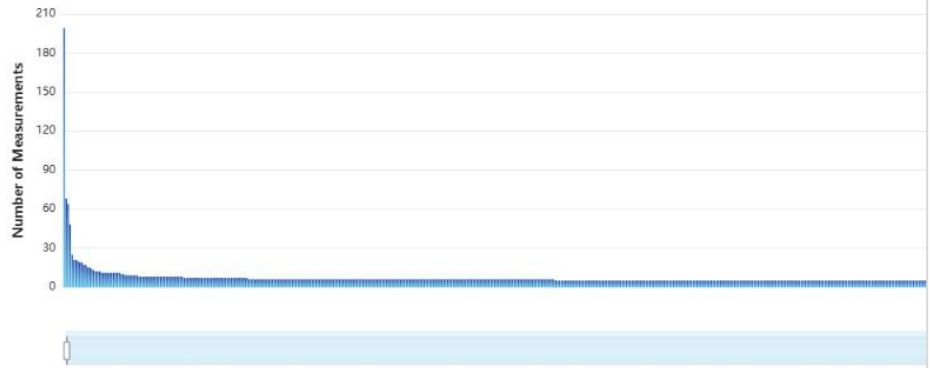
相關配體與藥理活性數據

藥理活性數據

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



Applied Filters (0)

Show Structures ON

	Ligand	Parameter	pvalue	Value	Function	Organism	Assay	Source
	1438423-22-3 5-[[(1*R*,2*S*)-2-Aminocyclohexyl]amino]-3-(3-pyridinylamino)-2-pyrazinecarboxamide	IC50	12.00	1×10^{-6} μM	Inhibitor	Homo sapiens	View	United States, US20130131040 A1 2013-05-23
	1438421-77-2 5-[[(1*R*)-1-(Aminocarbonyl)propyl]amino]-3-(2,1-benzisothiazol-3-ylamino)-2-pyraz...	IC50	12.00	1×10^{-6} μM	Inhibitor	Homo sapiens	View	United States, US20130131040 A1 2013-05-23
	1438422-34-4 5-[[(1*R*,2*S*)-2-Aminocyclohexyl]amino]-3-[(3-methyl-5-isothiazolyl)amino]-2-pyrazi...	IC50	12.00	1×10^{-6} μM	Inhibitor	Homo sapiens	View	United States, US20130131040 A1 2013-05-23
	1438420-30-4 5-[[(1*R*)-1-(Aminocarbonyl)-3,3-difluoropropyl]amino]-3-[(3,4-dimethylphenyl)amin...	IC50	12.00	1×10^{-6} μM	Inhibitor	Homo sapiens	View	United States, US20130131040 A1 2013-05-23

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...
Metabolites: 2 | Proteins: 581

2
62996-74-1
Staurosporine
Metabolites: 4 | Proteins: 1,024

3
1370261-96-3
2-[[(1*R*,2*S*)-2-Aminocyclohexyl]amino]-4-[[3-(2*H*-1,2,3-triazol-2-yl)phenyl]amino]-...
Metabolites: 0 | Proteins: 27

4
152459-95-5
Imatinib
Metabolites: 1 | Proteins: 676

5
544444-90-8
(-)-*cis*-Tetrahydroisohumulone

6
732983-37-8
2-[[7-(3,4-Dimethoxyphenyl)imidazo[1,2-*c*]pyrimidin-5-yl]amino]-3-pyridinecarboxa...

7
1240390-27-5
2-[[(3*R*,4*R*)-3-Aminotetrahydro-2*H*-pyran-4-yl]amino]-4-[(4-methylphenyl)amino]-5-p...

8
841290-81-1
Tamatinib

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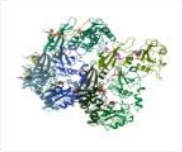
蛋白相關疾病資訊



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 metallopeptidase inhibitor 1, Solute carrier family 22 member 4, Tumor necrosis factor, Matrix metallopeptidase 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 Ia, 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

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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:(C (talin)2:(Syk{pY})2 + 2 NDP	Biology (2002), 157(2), 265-275
	Fibrinogen + 2 alpha IIb beta3:Csk:Src{pY529	Biology (2002), 157(2), 265-275
	SLP-76 + NTP --Fibrinogen:(alpha IIb beta3)2:	916-5923 963-5971
	vasp + SLAP-130{p} + SLP-76{p} <==> vasp:SL	ogical Chemistry (2001), 276(8), 5916-5923
	Fibrinogen:(alpha IIb beta3)2:(Src{pY529})2 --	ogical Chemistry (1998), 273(48), 31890-31900
	VAV1{pY}:SLP-76{p}:Nck-1 + PAK1 + Rac1:GTP	ogical Chemistry (1996), 271(42), 25746-25749 ogical Chemistry (1995), 270(49), 29071-4 ogical Chemistry (2001), 276(8), 5916-5923

Coordinate interactions of Csk, Src, and Syk kinases with αIIbβ3 initiate integrin signaling to the cytoskeleton

4 | 347 | Citation Map

In this Reference
- Concepts
- Substances
- Cited Documents

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

DOI: 10.1083/jcb.200112113

Integrins regulate cell adhesion and motility through tyrosine kinases, but in constitutively with integrin αIIbβ3 in platelets. Platelet adhesion to fibrinoge localized to filopodia and cell edges. Csk, which neg. regulates Src by phosp fibrinogen binding caused Csk to dissociate from αIIbβ3, concomitant with dephosphorylation of Src Tyr-529 and phosphorylation of Src activation loop Tyr-418. In contrast to the behavior of Src and Csk, Syk was associated with αIIbβ3 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 αIIbβ3, 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

一鍵連結到SciFinder文獻詳情頁

Publication Information • Journal — View Less

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 CAplus and MEDLINE	Division of Vascular Biology, Department of Cell Biology The Scripps Research Institute La Jolla, California 92037 United States	Rockefeller University Press	English

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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 | Draw

← 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-reac
- Erb-b2
- Microt tau
- Estrog
- 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-bispho sphate 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

疾病簡介

生物標誌物

相關靶點與配體

Sort: Relevance

	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	7,479	1M
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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 metallopeptidase domain 10, View All	2,937	430K

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疾病詳情頁與相關藥物資訊

相關生物標誌物、藥理活性數據、配體與靶點

Alzheimer's disease

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
Alzheimers dementia
Early onset Alzheimer's disease
Intermediate-stage Alzheimer's disease
Late onset Alzheimer's disease
View Less

歸一化的疾病同義詞清單

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) (), 5(2), 88-98
23173-12-8 *rel*-(4a*R*,6*S*,8a*R*)-4a,5,9,10,11,12-Hexahydro-3-methoxy-11-methyl-6*H*-benzofuro[3a,3...	Palliative	Approved	Source
86332-23-2 1,2,3-Propanetriol, 2-(dihydrogen phosphate), monopotassium salt	Palliative	Approved	Source
120011-70-3 Donepezil hydrochloride	Palliative	Approved	Source

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疾病與生物標誌物

AI Table Summarization

AI總結

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

Alzheimer's disease

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

Applie

生物標誌物 | 參數 | 實驗說明 | 有機體 | 文獻來源

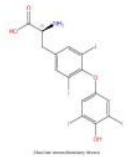
Show Filters | Summarize

Biomarker	Gene	Category	Parameter	Measurement	Organism	Assay	Source
(-)-Thyroxine	-	Diagnostic	Biomarker level	Mean free Thyroxine (FT4) level was observed in 40 patients with alzheimer's disease with blunted TSH response which is significantly (P< 0.01) more severely demented when compared to patients with non	Human	View	Biological psychiatry (), 30(6), 567-76
(+)-Aldosterone	-	Pharmacodynamic/resp				ew	Health Evaluation in African Americans Using RAS Therapy
(25*R*)-26-Hydroxycholesterol	-	Prognostic				ew	Brain Communications (2023), 5(5), 1-14
[Pyruvate dehydrogenase (acetyl-transferring)] kinase isozyme 1, mitochondrial	-	Diagnostic				ew	Journal of Biological Chemistry (2012), 287(44), 37245-37258

(-)-Thyroxine Detail

← Prev (1 of 9,000) Next →

Biomarker
51-48-9



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

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

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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）**

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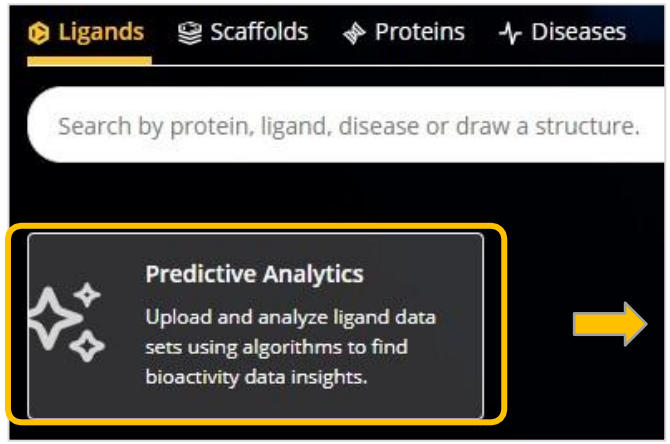
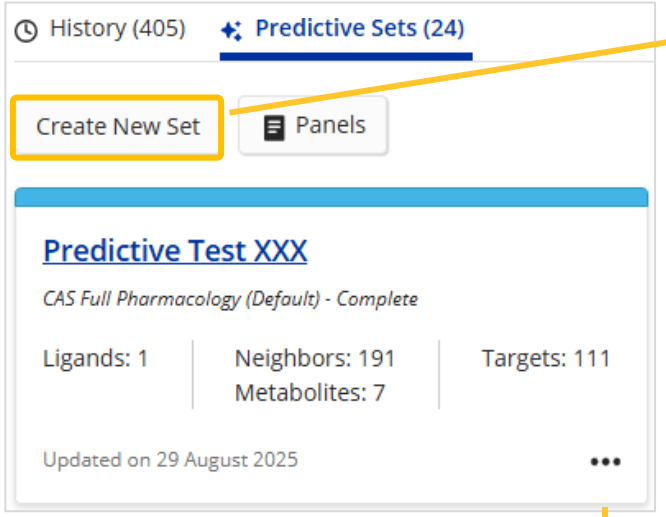
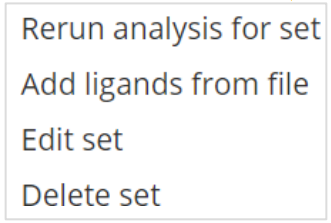
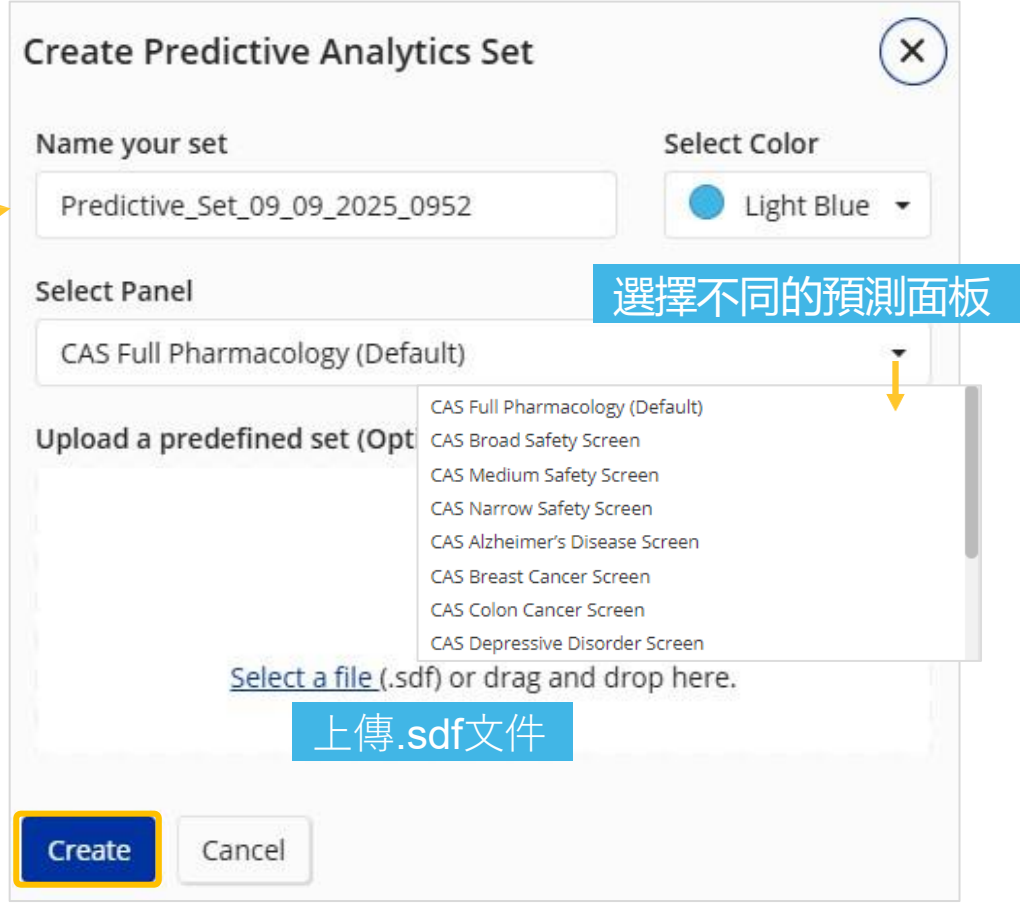
Predictive Analytics：通過演算法預測配體對不同靶點的生物活性數據









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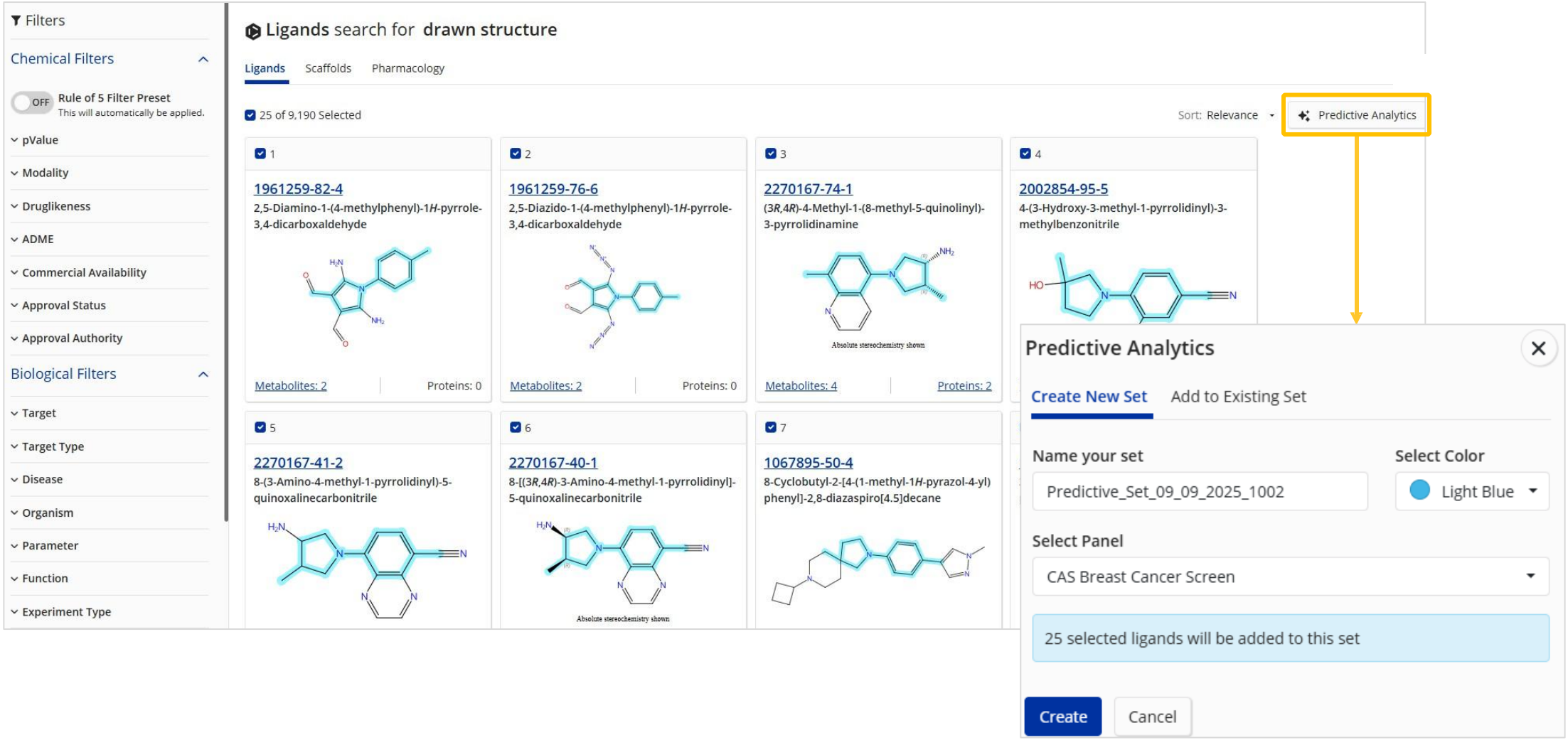
可從檢索結果集中添加配體結構



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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 Scree

Ligands: 25

Updated on 09 Septem

Panels

+ Create New Panel

Search panels by name...

点击查看详细靶点名称列表

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

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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
CAS Bi	
CAS M	

Create Predictive Analytics Panel

Panel Name

Predictive_Panel_Test

Description (Optional)

Cancel | Create Panel

Predictive_Panel_Test

可自定义面板名称

Targets to Include in Panel

Target	Organism	Uniprot ID
Prostaglandin F2-alpha receptor	Felis catus	6L9K4
Gag-pol polyprotein	Escherichia coli	A0A0A0F4Y0
Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform	Rattus norvegicus	A0A0G2K344
Dihydroorotate dehydrogenase (quinone)	Plasmodium falciparum Dd2	A0A0L7M6L3
Bifunctional dihydrofolate reductase-thymidylate synthase	Cryptosporidium hominis	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

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

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)

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生物活性預測結果

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

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。

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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
- 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

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https://biofinder.cas.org/

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Between problems and progress are connections that matter

謝謝！

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