

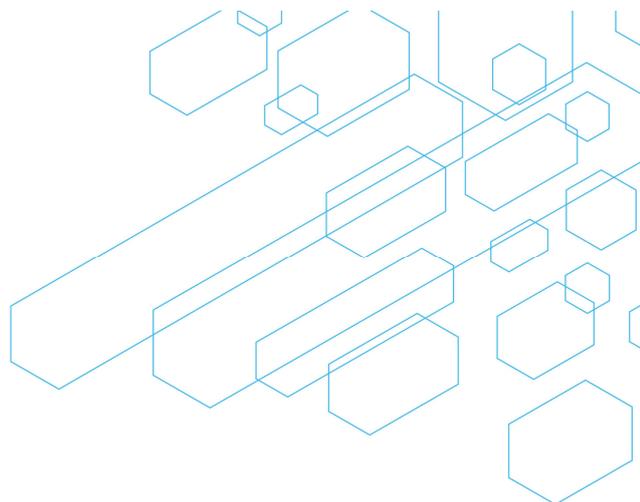
CAS BIOFINDER™ クイックガイド

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目次

- CAS BioFinder の概要
- 検索の流れ
- Ligands 検索
- Scaffolds 検索
- Proteins 検索
- Diseases 検索
- Predictive Analytics



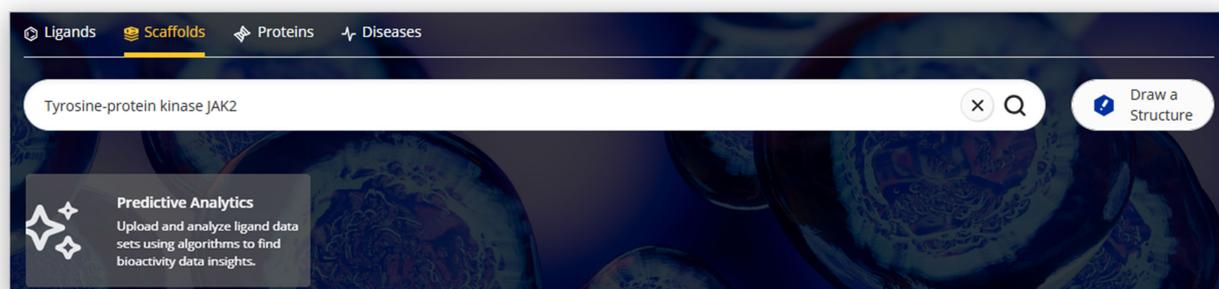
CAS BIOFINDER の概要

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CAS BioFinder とは

創薬に関する情報を一元的に検索できるツール



- 雑誌論文や特許文献、パブリックデータベースからライフサイエンスデータを標準化して収録
- キーワード・構造情報からリガンド、スキヤフォールド、タンパク質、疾患の情報を検索
- リガンドの薬理活性や代謝物、疾患のバイオマーカー等の関連情報にシームレスにアクセス
- AI を使った既知・新規リガンドのターゲットに対する活性の予測

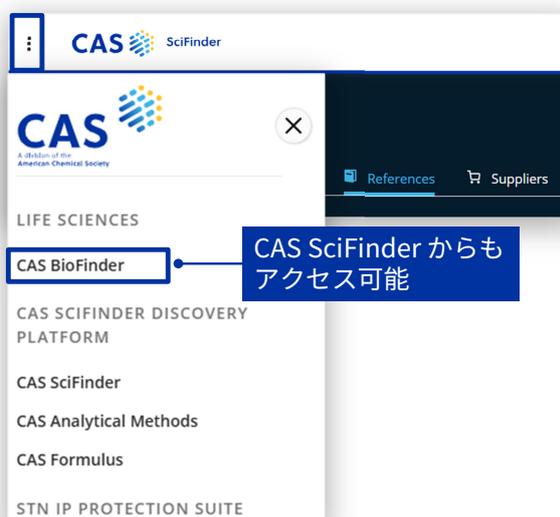
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検索の流れ

アクセス方法

<https://biofinder.cas.org>



検索初期画面

リガンド検索
スキヤフォールド検索
タンパク質検索
疾患検索

化学構造から検索する

Ligands Scaffolds Proteins Diseases 検索タイプの切り替え

Tyrosine-protein kinase JAK2

Draw

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

標的タンパク質、リガンド、疾患名から検索する

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(参考) 化学構造からの検索

いくつかの置換基パターンを指定した柔軟な検索も可能

CAS Draw search for Ligands

検索タイプの切り替え

Ligands Scaffolds Proteins Diseases

Enter a CAS Registry Number, SMILES, or InChI...

R1

-CN、-OCH₃、-C(O)NH₂

Molecular Formula: Formula is not available

Zoom: 110%

Search Cancel

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LIGANDS 検索

9

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回答一覧画面

Ligands search for Tyrosine-protein kinase JAK2

Ligands Scaffolds Pharmacology **表示項目の切り替え (p18、p24)**

44,854 Results

詳細の表示 (p13)

Item	Chemical Name	Metabolites	Targets
1	62996-74-1 Stauroporine	4	938
2	284461-73-0 Sorafenib	10	746
3	149647-78-9 Vorinostat	11	204
4	15249-... Imatinib	4	686

Sort: Relevance **回答の並べ替え** Predictive Analyt...

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

10

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回答の絞り込み (1/2)

Chemical Filters

Rule of 5 Filter Preset

リピンスキーの5つのルールに基づいて、8つの異なるDruglikenessおよびADMEフィルターを所定の値に設定する*

ADME

Partition Coefficient (logP)
Solubility (logS)
Blood-Brain Barrier Permeability (logBB)
Permeability Glycoprotein (Pgp)
Polar Surface Area (PSA) (Å²)
Plasma Protein Binding (PPB)

Commercial Availability

市販の有無

Chemical Filters

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

^ pValue

1.00 to 14.00

1.00 to 14.00

Reset Filter Apply

▼ Druglikeness

▼ ADME

▼ Commercial Availability

pValue

IC50などの活性値の負の対数をモル単位で表したもの

Druglikeness

Hydrogen Bond Acceptors
Hydrogen Bond Donors
Freely Rotatable Bonds
Molecular Weight (g/mol)
Molar Refractivity (m³/mol)
Number of Atoms

* 設定される値は Help 参照

https://cas-biofinder.zendesk.com/hc/en-us/articles/26034817456013-Scaffold-Results-Overview#h_01HWVEVBX09Q9R30YVFG3V1G

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回答の絞り込み (2/2)

Biological Filters、Source Filters

Biological Filters

^ Target

Tyrosine-protein kinase JAK2
 Tyrosine-protein kinase JAK1
 Tyrosine-protein kinase JAK3
 Non-receptor tyrosine-protein kinase TYK2
 Epidermal growth factor receptor

[View All](#) Apply

▼ Target Type

▼ Disease

▼ Organism

▼ Parameter

▼ Function

▼ Experiment Type

Target

ターゲット

Target Type

ターゲットタイプ (タンパク質、細胞株等)

Disease

疾患

Organism

生物種

Parameter

パラメータ (IC50、Ki 等)

Function

機能 (Inhibitor、Agonist 等)

Experimental Type

実験の種類 (In vivo、In vitro 等)

Source Filters

▼ Document Type

▼ Publication Year

▼ Language

Document Type

資料種類

Publication Year

発行年

Language

言語

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回答の詳細画面 (1/5)

関連情報にスムーズにアクセスできる

Knowledge Graph*

View in CAS SciFinder

当物質の文献情報

当物質の反応情報

逆合成解析

予測解析機能 (p34)

スキヤフォールドへのアクセス View in CAS SciFinder (物質情報)

各タブの説明は p13

CAS DRUG INTELLIGENCE

Monomethyl Auristatin E (MMAE) is an antimitotic agent which inhibits cell division by blocking the polymerization of tubulin. Monomethyl Auristatin E is the synthetic analog of the amineoepilastic natural product Dolastatin 10, cannot be used as a drug itself. Monomethyl Auristatin E is commonly co...

STATUS

Approval Status: Designated
Approval Authority: Other
Approval Year: Unknown
Originator: Seattle Genetics

INDICATIONS

Cancer
Modality: Primary
Highest Phase: Basic research
Source

PRIMARY TARGET

Tubulin
Function: Inhibitor
Source

H bond acceptor*	H bond donor*	Molecular weight (g/mol)	Molar refractivity (m ³ /mol)	Number of atoms	Freely rotatable bonds*	logP*	logS	logDD	Polar surface area (Å ²)*	Plasma protein binding	Permeability: glycoprotein
12	4	717.98	198.45	51	20	3.822	-5.69	-0.85	149.54	82.96	1

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

*Knowledge Graph (<https://cas-biofinder.zendesk.com/hc/en-us/articles/23287951441037-Ligand-Detail-Overview>)

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回答の詳細画面 (2/5)

表示タブは 10 種類

Monomethylauristatin E

CAS Registry Number: 474645-27-7

2,295 856 Retrosynthesis Knowledge Graph Predictive Analytics ...

Summary Pharmacology ADME Toxicology Proteins (13) Diseases (10) Related Immunotherapeutics (734) Chemical Space Metabolites (11) Similar Ligands (10K)

- Summary : 概要 (p15)
- Pharmacology : 薬理学的データ (p24)
- ADME : 薬物動態 *
- Toxicology : 毒性*
- Proteins : 標的タンパク質 (p26)
- Disease : 疾患 (p30)
- Related Immunotherapeutics : 関連する抗体医薬品 (p16)
- Chemical Space* : 着目しているリガンドと類似化合物の物理化学的パラメータを散布図で表示
- Metabolites : 代謝物
- Similar Ligands : 類似の構造を持つリガンド*

*<https://cas-biofinder.zendesk.com/hc/en-us/articles/23287951441037-Ligand-Detail-Overview>

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⑤回答の詳細画面 (3/5)

Summary タブでリガンドの概要を把握できる

CAS DRUG INTELLIGENCE
承認済みの医薬品である場合に
医薬品の概要を表示

物理化学的パラメータ

H bond acceptors*	H bond donors*	Molecular weight (g/mol)	Molar refractivity (m ³ /mol)	Number of atoms	Freely rotatable bonds*	logP*	logS	logBB	Polar surface area (Å ²)	Plasma protein binding	Permeability glycoprotein
12	4	717.98	198.45	51	20	3.822	-5.69	-0.85	149.54	82.96	1

CAS DRUG INTELLIGENCE
Monomethyl Auristatin E (MMAE) is an antimitotic agent which inhibits cell division by blocking the polymerization of tubulin. Monomethyl Auristatin E is the synthetic analog of the antineoplastic natural product Dolastatin 10. cannot be used as a drug itself. Monomethyl Auristatin E is commonly co... [View More](#)

STATUS	Approval Status: Designated Approval Authority: Other Approval Year: Unknown Originator: Seattle Genetics
INDICATIONS	Cancer Modality: Primary Highest Phase: Basic research Source
PRIMARY TARGET	Tubulin Function: Inhibitor Source

回答の詳細画面 (4/5)

Related Immunotherapeutics タブは指定のリガンドを含む抗体医薬品を確認できる

**Antibody、Antigen、Payload
Therapeutic Target、
Drug-Antibody Ratio、Linker、Method**

Adalimumab

Antibody	Adalimumab
Antigen	Tumor necrosis factor (TNF)
Payload	Monomethyl auristatin E
Therapeutic Target	Microtubule
Drug-Antibody Ratio	3.5-4
Linker	Adalimumab-Compound 69 linker
Method	Random conjugation through reduced inter-chain cysteines.

Trastuzumab

Antibody	Trastuzumab
Antigen	Receptor tyrosine-kinase erbB-2 (ERBB2)
Payload	Monomethyl auristatin E
Therapeutic Target	Microtubule
Drug-Antibody Ratio	2
Linker	WO201708995A1_ADC11 linker

ペイロードとして MMAE を含む

回答の詳細画面 (5/5)

Metabolites タブでは既知 (Known) もしくは予測の代謝物を確認できる

Monomethylauristatin E
CAS Registry Number: 474645-27-7

2,284 847 Retrosynthesis Knowledge Graph Predictive Analytics

Summary Pharmacology ADME Toxicology Proteins (13) Diseases (10) Related Immunotherapeutics (734) Chemical Space **Metabolites (11)** Similar Ligands (10K)

0.15 0.17 0.21 0.90

0.25 0.13

予測の場合は信頼度のスコアが表示され
既知の場合は Known と表示される

SCAFFOLDS 検索

回答一覧画面

リガンドの構造から鎖の置換基を取り除いた骨格構造で表示

Scaffolds search for **tyrosine-protein kinase jak2**

15,366 Results

1 Ligands: 54K Proteins: 5,767

2 Ligands: 3,324 Proteins: 1,447

3 Ligands: 7,127 Proteins: 1,181

4 Ligands: 6,706 Proteins: 1,237

5 Ligands: 2,582 Proteins: 1,013

6 Ligands: 3,787 Proteins: 720

回答の並べ替え

Sort: Relevance

- Relevance
- Number of Ligands: Ascending
- Number of Ligands: Descending
- Number of Proteins: Ascending
- Number of Proteins: Descending

リガンドのいずれかが作用するターゲットの数

表示のスキフォールドに分類されるリガンドの数

P11 - 12

回答の詳細画面

選択したスキフォールドに分類されるリガンドの一覧が表示される

BNHMHILVWPJP-UHFFFAOYSA-N

1 of 12 Scaffolds

2 62996-74-1 Staurosporine

3 160335-45-5 (9R,10S,11S,13S)-2,3,10,11,12,13-Hexahydro-10-methoxy-9-methyl-11-(methylamino)-...

4 159404-54-3 9,13-Epoxy-1H,9H-diindolo[1,2,3-f:4',5'-g]azorin-...

5 112953-11-4 7-Hydroxystaurosporine

6 159404-45-2 9,13-Epoxy-1H,9H-diindolo[1,2,3-fh:3',2',1'-lm]pyrrolo[3,4-j]1,7-benzodi-azoni-...

7 121569-61-7 (3S,9S,10R,11R,13R)-2,3,10,11,12,13-Hexahydro-3-hydroxy-10-methoxy-9-methyl-11-(methylamino)-9,13-epoxy-1H,9H-diindolo[1,2,3-f:4',5'-g]azorin-...

8 2449215-18-1 2,3,10,11,12,13-Hexahydro-10-methoxy-11-(methylamino)-9,13-epoxy-1H,9H-diindolo[1,2,3-f:4',5'-g]azorin-...

9 112953-11-4 7-Hydroxystaurosporine

10 159404-45-2 9,13-Epoxy-1H,9H-diindolo[1,2,3-fh:3',2',1'-lm]pyrrolo[3,4-j]1,7-benzodi-azoni-...

11 121569-61-7 (3S,9S,10R,11R,13R)-2,3,10,11,12,13-Hexahydro-3-hydroxy-10-methoxy-9-methyl-11-(methylamino)-9,13-epoxy-1H,9H-diindolo[1,2,3-f:4',5'-g]azorin-...

12 2449215-18-1 2,3,10,11,12,13-Hexahydro-10-methoxy-11-(methylamino)-9,13-epoxy-1H,9H-diindolo[1,2,3-f:4',5'-g]azorin-...

回答の絞り込み (p21)

回答の並べ替え

Sort: Relevance

- Relevance
- CAS RN: Ascending
- CAS RN: Descending
- Number of Proteins: Ascending
- Number of Proteins: Descending
- Number of Metabolites: Ascending
- Number of Metabolites: Descending
- Suppliers

p22 p34

回答の絞り込み

R-Groups フィルターで置換基を解析、限定できる

Scaffold Summary

Filters

Chemical Filters

Rule of 5 Filter Preset
This will automatically be applied.

R-Groups

R1 2 R2 5 R3 2
R4 2 R5 2 R6 2
R7 3 R8 46 R9 6
R10 3 R11 3

R8には46種類の置換基が存在する

R8 for BNHMHILVWPPJP-UHFFFAOYSA-N (46)

30 Ligands 19 Ligands 3 Ligands 2 Ligands
5 Ligands 5 Ligands 3 Ligands 2 Ligands
2 Ligands 2 Ligands 2 Ligands 2 Ligands

R8に水酸基を有するリガンドに限定

Matched Molecular Pairs Analysis (MMPA) (1/2)

選択したスキヤフォールドの構造活性相関を視覚的に解析する機能

BNHMHILVWPPJP-UHFFFAOYSA-N
Murcko scaffold InChI Key

← Prev (3 of 1,647) Next →

Ligands Pharmacology Similar Scaffolds

119 Results Sort: Relevance Get MMPA Predictive Analytics

Select a Target for Matched Molecular Pairs Analysis (MMPA)

Protein kinase c

Target

Protein kinase C alpha type
Protein kinase C
Protein kinase C theta type
Protein kinase C beta type
Protein kinase C delta type
Protein kinase C epsilon type
Protein kinase C eta type
Protein kinase C gamma type

活性を比較するターゲットを選択する

Select one R-Group Cluster to Visualize

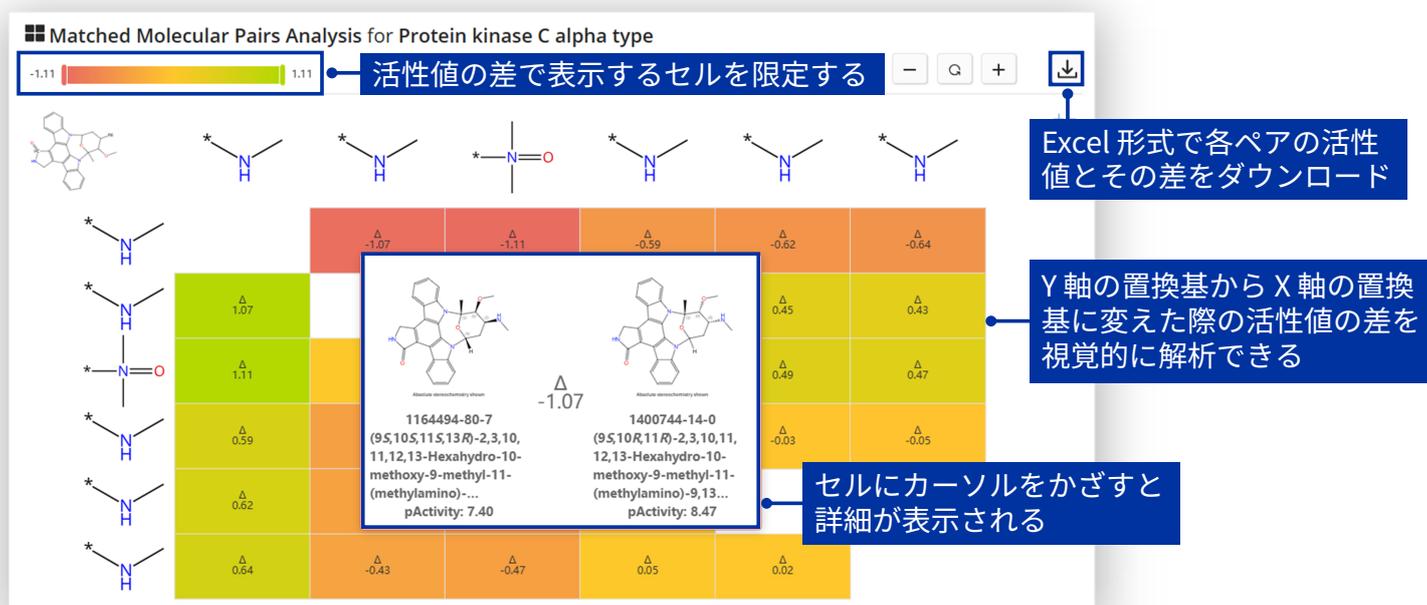
36 Matched Molecular Pairs 15 Matched Molecular Pairs 15 Matched Molecular Pairs 15 Matched Molecular Pairs

活性を比較する置換位置を選択する

← Prev 1 2 Next → Show 10 per page

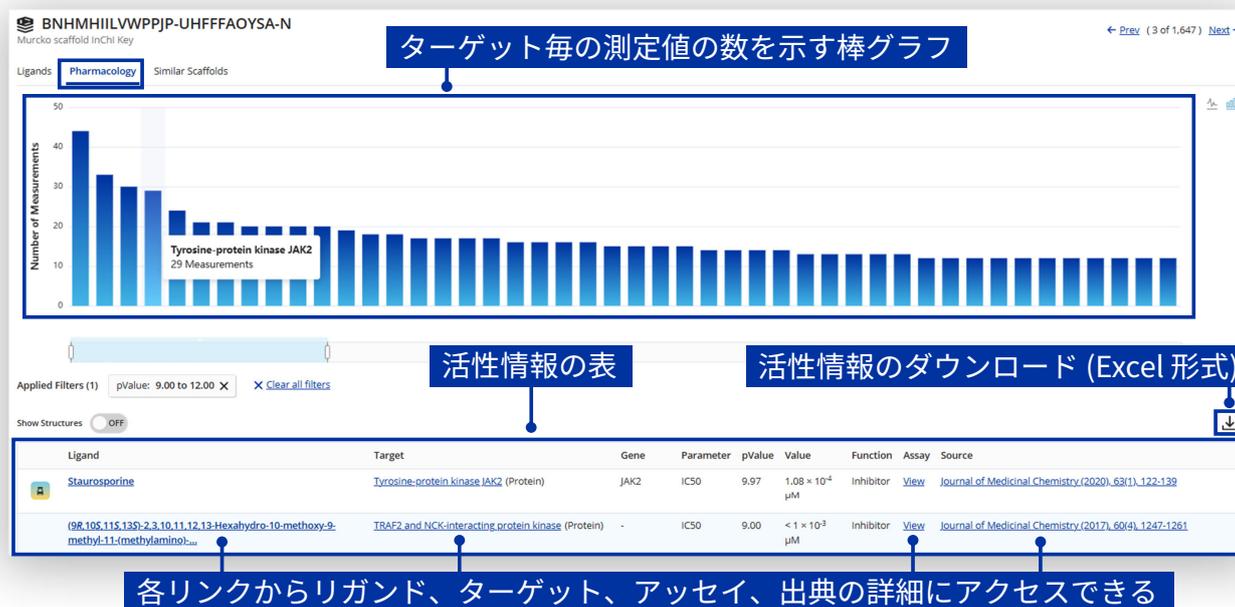
Previous Submit 解析結果 → p 24

Matched Molecular Pairs Analysis (MMPA) (2/2)



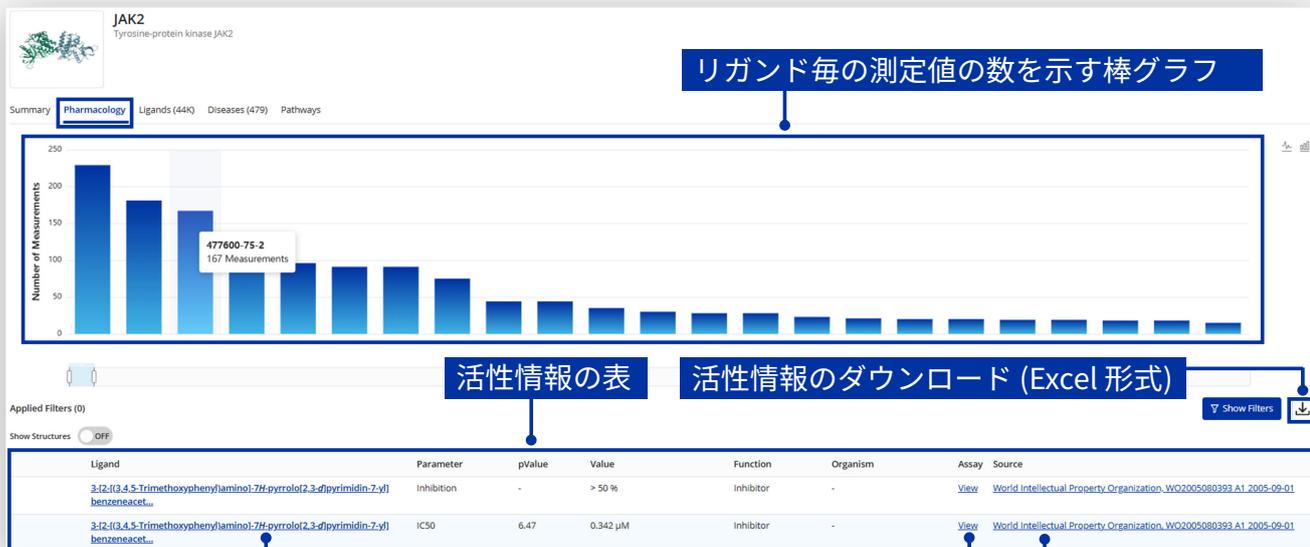
Pharmacology タブ

Scaffolds、Ligands、Diseases の場合



Pharmacology タブ

Proteins の場合



リガンド毎の測定値の数を示す棒グラフ

活性情報の表

活性情報のダウンロード (Excel 形式)

各リンクからリガンド、アッセイ、出典の詳細にアクセスできる

PROTEINS 検索

Proteins の検索結果画面

検索例: Tyrosine-protein kinase JAK2

Proteins search for Tyrosine-protein kinase JAK2

Proteins Pharmacology **Pharmacology タブ (p.24)**

4 Results Sort: Relevance View: List

Protein	Organism	24K	271
1 JAK2 Tyrosine-protein kinase JAK2	Homo sapiens	24K	271
2 JAK2 Tyrosine-protein kinase JAK2	-	23K	421
3 jak2 Tyrosine-protein kinase JAK2	Mus musculus	225	12
4 Jak2 Tyrosine-protein kinase JAK2	Rattus norvegicus	1	2

タンパク質の詳細画面 → p.28

関連のリガンド情報の検索

関連の疾患情報の検索

Proteins の詳細画面 (1/2)

Summary

関連のリガンドと疾患情報

JAK2 Tyrosine-protein kinase JAK2

Summary Pharmacology Ligands (44K) Diseases (479) Pathways **関連のパスウェイ情報 (p.29)**

p.24

The structural basis of Janus Kinase 2 inhibition by a potent and specific pan-Janus kinase inhibitor



生物種を選択

Organism: Homo sapiens (selected), Mus musculus, Rattus norvegicus, unspecified

in-receptor and growth factor signalling. The primary isoform of this protein has main that is required for erythropoietin receptor association, an SH2 domain that binds STAT transcription factors, a pseudokinase and tyrosine kinase domain. Cytokine binding induces autophosphorylation and activation of this kinase. This kinase then recruits and activates transcription factors (STAT) proteins. Growth factors like TGF-beta 1 also induce phosphorylation and activation of this kinase and translocation of downstream STAT proteins to the nucleus where they influence gene transcription. Mutations in this gene are associated with numerous inflammatory diseases and malignancies. This gene is a downstream target of the pleiotropic cytokine IL6 that is produced by B cells, T cells, dendritic cells and macrophages to produce an immune response or inflammation. Dysregulation of the IL6/JAK2/STAT3 signalling pathway produces increased cellular proliferation and myeloproliferative neoplasms of hematopoietic stem cells. A nononymous mutation in the pseudokinase domain of this gene disrupts the domains inhibitory effect and results in constitutive tyrosine phosphorylation activity and hypersensitivity to cytokine signalling. This gene and the IL6/JAK2/STAT3 signalling pathway is a therapeutic target for the treatment of excessive inflammatory responses to viral infections. Alternative splicing results in multiple transcript variants encoding distinct isoforms. [provided by RefSeq, Jul 2020]

Identifier	Method	Resolution	Chain	Positions	Source
2B7A	X-Ray	2.00 Å	A/B	840 - 1132	PDB
2W11	X-Ray	2.60 Å	A/B	835 - 1132	PDB
2XA4	X-Ray	2.04 Å	A/B	835 - 1132	PDB
3E62	X-Ray	1.922 Å	A	839 - 1131	PDB
3E63	X-Ray	1.9 Å	A	839 - 1131	PDB
3E64	X-Ray	1.8 Å	A	839 - 1131	PDB
3EUP	X-Ray	2.40 Å	A/B	840 - 1132	PDB
3I07	X-Ray	2.600 Å	A	842 - 1132	PDB

Protein Data Bank 由来の 3D モデルの情報

Proteins の詳細画面 (2/2)

Pathways

JAK2
Tyrosine-protein kinase JAK2

Summary Pharmacology Ligands (44K) Diseases (479) **Pathways**

Pathway	Reaction	Source
PD-L1 activation pathway	IKK-alpha(p):IKK-beta(pS177){pS181}:(IKK-gamma)2:TRADD:TRAF2(ub{K63}(n)):RIP(ub{K63}(n)K377):tab2:tab3:tab1:TAK1 -> IKK-alpha(p):IKK-beta(pS177){pS181}:(IKK-gamma)2 + TRADD:TRAF2(ub{K63}(n)):RIP(ub{K63}(n)K377):tab2:tab3:tab1:TAK1	Trends in Biochemical Sciences (2005), 30(1), 1-4
	diacyl lipopeptide:TLR2:TLR6:GP4:TIRAP:MyD88:IRAK-4(p):IRAK-2(p):IRAK-1(pT209) + ATP -> diacyl lipopeptide:TLR2:TLR6:GP4:TIRAP:MyD88:IRAK-4(p):IRAK-2(p):IRAK-1(pT209){pT387} + ADP	Nature Immunology (2010), 11(5), 373-384
	EGF:(EGFR)2 + ATP -> EGF:(EGFR(pY))2 + ADP	EMBO Journal (2000), 19(13), 3159-3167 Molecular Biology of the Cell (2002), 13(7), 2547-2557
	2 STAT3(pY705){pS727} <=> (STAT3(pY705){pS727})2	Nature Reviews Cancer (2014), 14(11), 736-746 Growth Factors (2018), 36(1-2), 1-14 Nucleic Acids Research (2024), 52(D1), D672-D678
	SHP-2(pY304){pY327} + Gab-1 + Grb-2 <=> SHP-2(pY304){pY327}:Gab-1:Grb-2	Journal of Biological Chemistry (1997), 272(2), 1032-1037
	Dvl + Fz:Wnt <=> Dvl:Fz + Wnt	Journal of Cell Science (2002), 115(21), 3977-3978
	diacyl lipopeptide:TLR2:TLR6:GP4 + TIRAP + MyD88 <=> diacyl lipopeptide:TLR2:TLR6:GP4:TIRAP:MyD88	Clinical Microbiology Reviews (2009), 22(2), 240-273
	EGF-ECD:(EGFR-p170(pY1016){pY1092}{pY1110}{pY1172}{pY1197})2:Grb-2:Sos1(pY):Ras-C(farC) (metC):GTP + p85:p110 <=> EGF-ECD:(EGFR-p170(pY1016){pY1092}{pY1110}{pY1172}{pY1197})2:Grb-2:Sos1(pY):H-Ras:GTP:p85:p110	Journal of Cell Biology (2002), 156(1), 125-136

CAS SciFinder の出典情報へのリンク



DISEASES 検索



Diseases の検索結果画面

検索例：Tyrosine-protein kinase JAK2

Diseases search for Tyrosine-protein kinase JAK2

473 Results

Disease	Description	Biomarkers
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
Alzheimer disease	Alzheimer disease is a neurodegenerative disease characterized by memory lapses, confusion, emotional instability results in progressive memory loss, impaired personality and mood starting and leads in advanced cases to a profound decline in cognitive and physical functioning and is marked histologically by the degeneration of brain neurons especially in the cerebral cortex and by the presence of neurofibrillary tangles and plaques containing beta-amyloid.	Apolipoprotein E, Fibrinogen alpha chain, Iset amyloid polypeptide, APP (rs199862130) polymorphism, Synuclein alpha, View All
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
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
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 domain containing protein tyrosine phosphatase 2, Insulin, Mechanistic target of rapamycin kinase, View All
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
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
Inflammation	Inflammation is a general symptom where there is a local response to cellular injury that is marked by capillary dilatation, leukocytic infiltration, redness, heat, pain, swelling, and often loss of function and that serves as a mechanism initiating the elimination of noxious agents and of damaged tissue.	Haptoglobin, Coagulation factor II thrombin receptor, Immediate early response 3, POU class 2 homeobox 2, Myosin light chain 4, View All

Answers can be sorted by: Relevance

- Number of Ligands: Ascending
- Number of Ligands: Descending
- Number of Proteins: Ascending
- Number of Proteins: Descending

関連のリガンド情報

関連のタンパク質情報



Diseases の詳細画面 (1/2)

Summary

関連のバイオマーカー情報 → p.33

Cancer

Summary **Biomarkers** **Pharmacology** **Ligands (966K)** **Proteins (7,169)** 関連のリガンド、タンパク質情報

A disease of cellular proliferation that is malignant and primary, characterized by uncontrolled cellular proliferation, local cell invasion and metastasis.

Synonyms

- Adult solid tumor
- Advanced and/or refractory solid tumors
- Advanced cancer
- Advanced malignant solid neoplasm
- Advanced neoplasms

[View More](#) ▾

External Links and Identifiers

- MESH: [D009369](#)
- NCI: [C9305](#)



Diseases の詳細画面 (2/2)

Biomarkers

Cancer

Summary **Biomarkers** Pharmacology Ligands (966K) Proteins (7,169)

AI によるバイオマーカーの要約機能*

Applied Filters (0) Show Filters Summarize Download

ダウンロード (Excel 形式)

Biomarker	Gene	Category	Parameter	Measurement	Organism	Assay	Source
BRCA1 DNA repair associated	BRCA1	Gene-disease association linked with genetic variation	Association score	0.3	Human	View	European Journal of radiology.0_1060_150-159
Neurotrophin 4	NTF4	Gene-disease association linked with genetic variation	Association score	0.1	Human	View	Oncology Letters (2018), 15(1), 1-5
Autophagy related 16 like 1	ATG16L1	Gene-disease association linked	Association	0.25	Human	View	Molecular Biology Reports

アッセイの詳細情報

CAS SciFinder の出典情報へのリンク

* <https://cas-biofinder.zendesk.com/hc/en-us/articles/37350782594317-Disease-Detail-Overview>

PREDICTIVE ANALYTICS

Predictive Analytics (1/4)

リガンドの活性値の予測機能

Ligands Pharmacology Similar Scaffolds

Applied Filters (1) pValue: 9.00 to 12.00 X Clear all filters

17 of 17 Selected Sort: Relevance Get MMPA Predictive Analytics p.36

1 2 3

解析するリガンドを選択する (ページ全体 or 個別)

Metabolites: 4 Proteins: 938

Metabolites: 5 Proteins: 536

Metabolites: 5 Proteins: 351

Predictive Analytics (2/4)

解析の開始

既存の解析セットへの追加

Predictive Analytics

Create New Set Add to Existing Set

Name your set Predictive_Set_07_02_2025_1707 Select Color Light Blue

Select Panel CAS Full Pharmacology (Default)

17 selected ligands will be added to this set

Create Cancel

解析セットの作成

パネル (活性値を予測するターゲットセット) の選択

Select Panel

- CAS Full Pharmacology (Default)
- 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

Run analysis now?

Would you like to run the analysis for "Predictive_Set_07_02_2025_1720" now? You will be notified of the progress when the process is complete as you continue to use CAS BioFinder.

Yes, run now 解析開始

Predictive Analytics (3/4)

結果の表示

The screenshot shows the 'Diseases' tab in the Predictive Analytics interface. A search bar is present with the text 'Search by protein, ligand, disease or draw a structure.' Below it, a 'Predictive Analytics' box contains the text: 'Upload and analyze ligand data sets using algorithms to find bioactivity data insights.' An arrow points from this box to the 'Predictive Sets' section. The 'Predictive Sets' section displays a list of sets with the following data:

Set ID	Status	Ligands	Neighbors	Metabolites	Targets	Updated
Predictive_Set_07_02_2025_1656	Complete	17	29	86	325	02 July 2025
Predictive_Set_04_23_2025_0919	Complete	70	573	297	189	03 June 2025
Predictive_Set_04_23_2025_1035	Ready	70	-	297	-	23 April 2025

* <https://cas-biofinder.zendesk.com/hc/en-us/articles/32589017148685-Create-Custom-Analytics-Panels>

Predictive Analytics (4/4)

Pharmacology

The screenshot shows the results for 'Predictive_Set_07_02_2025_1656' in the 'Pharmacology' category. The 'Show Structures' toggle is turned OFF. The results are displayed in a table:

Ligand	Target	Known pAct	Predicted pAct	Confidence	Method
2449215-18-1	Tyrosine-protein kinase JAK2 (Homo sapiens)	9.26	8.53	0.68	●●●●●●
918327-50-1	Tyrosine-protein kinase JAK2 (Homo sapiens)	-	8.48	0.68	●●●●●●
125035-83-8	Tyrosine-protein kinase JAK2 (Homo sapiens)	-	8.47	0.6	●●●●●●
2566600-13-1	Tyrosine-protein kinase JAK2 (Homo sapiens)	-	8.46	0.62	●●●●●●
159404-45-2	Tyrosine-protein kinase JAK2 (Homo sapiens)	-	8.41	0.57	●●●●●●

* <https://cas-biofinder.zendesk.com/hc/en-us/articles/26239797361805-Predictive-Analytics-Results-Pharmacology>



JAICI ヘルプデスク

0120-003-462 (平日 9:00-12:00 / 13:00-17:00)

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