

DLiP 1.0

Database of Chemical Library for Protein-Protein Interaction

User Manual

～ ユーザーマニュアル ～

2020/04/01

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謝 辞

本データベースは、国立研究開発法人 日本医療研究開発機構(AMED) 創薬基盤推進研究事業における「PPI 界面三次元構造に基づく PPI 化合物ライブラリー (研究代表者: ペプチドリーム株式会社 古谷利夫)」の成果物の一つです。

本データベースは、慶應義塾大学薬学部、ペプチドリーム株式会社、
医薬基盤・健康・栄養研究所によって共同開発されました。

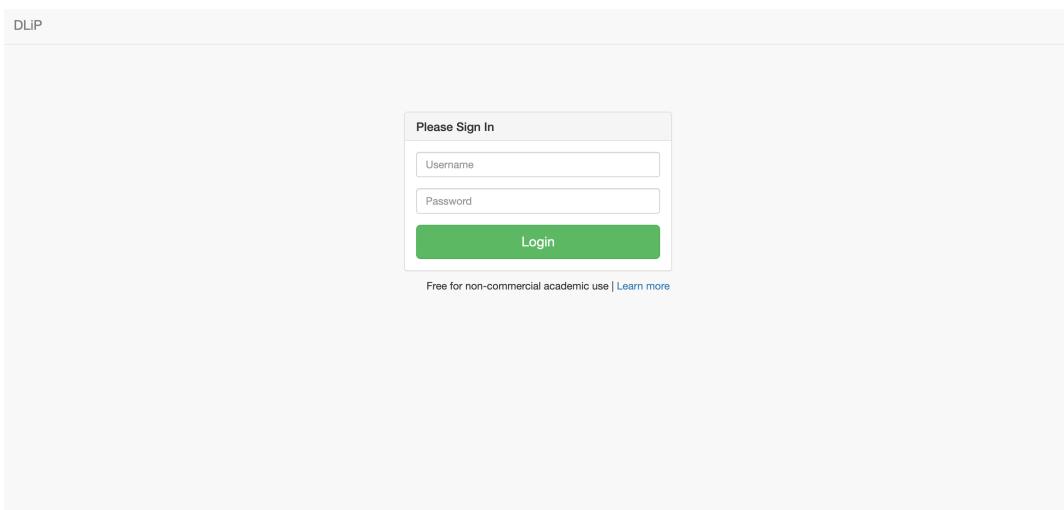
すべての関係者のご協力に感謝を申し上げます。

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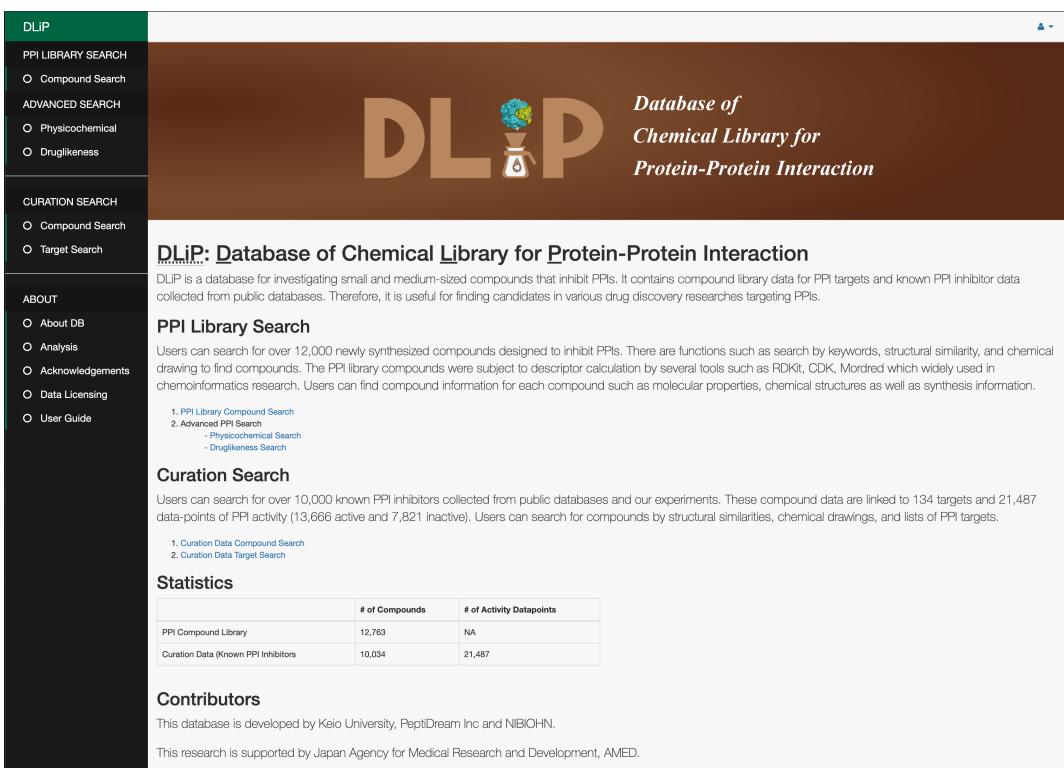
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1. ログイン

ユーザ名およびパスワードを入力する。新規ユーザの作成はシステム管理者に依頼すること。



ログインが完了し、トップページに遷移する。



DLIP

PPI LIBRARY SEARCH

- Compound Search

ADVANCED SEARCH

- Physicochemical
- Druglikeness

CURATION SEARCH

- Compound Search
- Target Search

ABOUT

- About DB
- Analysis
- Acknowledgements
- Data Licensing
- User Guide

DLIP: Database of Chemical Library for Protein-Protein Interaction

DLIP is a database for investigating small and medium-sized compounds that inhibit PPIs. It contains compound library data for PPI targets and known PPI inhibitor data collected from public databases. Therefore, it is useful for finding candidates in various drug discovery researches targeting PPIs.

PPI Library Search

Users can search for over 12,000 newly synthesized compounds designed to inhibit PPIs. There are functions such as search by keywords, structural similarity, and chemical drawing to find compounds. The PPI library compounds were subject to descriptor calculation by several tools such as RDKit, CDK, Mordred which widely used in chemoinformatics research. Users can find compound information for each compound such as molecular properties, chemical structures as well as synthesis information.

1. PPI Library Compound Search
2. Advanced PPI Search
- Physicochemical Search
- Druglikeness Search

Curation Search

Users can search for over 10,000 known PPI inhibitors collected from public databases and our experiments. These compound data are linked to 134 targets and 21,487 data-points of PPI activity (13,666 active and 7,821 inactive). Users can search for compounds by structural similarities, chemical drawings, and lists of PPI targets.

1. Curation Data Compound Search
2. Curation Data Target Search

Statistics

	# of Compounds	# of Activity Datapoints
PPI Compound Library	12,763	NA
Curation Data (Known PPI Inhibitors)	10,034	21,487

Contributors

This database is developed by Keio University, PeptiDream Inc and NIBIOHN.

This research is supported by Japan Agency for Medical Research and Development, AMED.

2. PPI Library Search

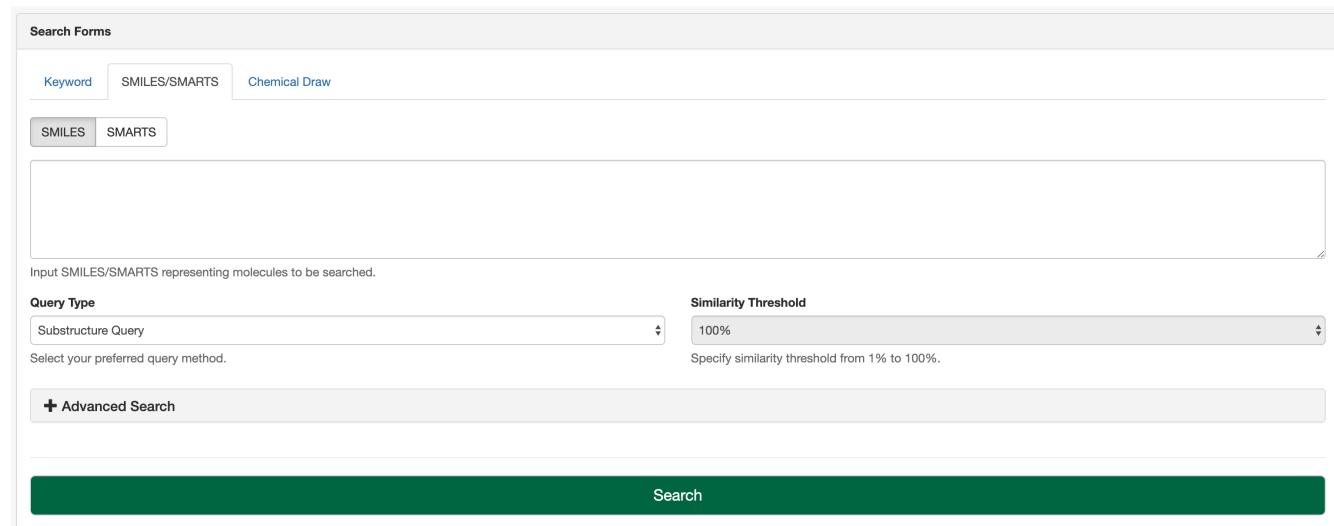
2.1. Compound Search

サイドメニューの **PPI LIBRARY SEARCH > Compound Search** またはトップページの **PPI Library Compound Search** からアクセスする。

2.1.1. 検索条件の指定

構造式

SMILES/SMARTS タブを選択することで構造式の入力フォームを表示する。



The screenshot shows the 'Search Forms' section of the PPI Library Compound Search interface. At the top, there are three tabs: 'Keyword' (selected), 'SMILES/SMARTS' (highlighted in red), and 'Chemical Draw'. Below these are two sub-tabs: 'SMILES' (selected) and 'SMARTS'. A large input field is present for entering SMILES/SMARTS strings. Below the input field, a placeholder text reads: 'Input SMILES/SMARTS representing molecules to be searched.' To the right of the input field, there are two dropdown menus: 'Query Type' (set to 'Substructure Query') and 'Similarity Threshold' (set to '100%'). A note below the threshold dropdown says: 'Specify similarity threshold from 1% to 100%.' At the bottom of the form is a large green 'Search' button.

構造式の形式(**SMILES** もしくは **SMARTS**)を選択し、構造式を入力する。

Keyword

SMILES/SMARTS

Chemical Draw

SMILES

SMARTS

O=C(NC1CCN(C(=O)Cn2c(C3CCOCC3)nc3cccc(F)c32)CC1)c1cccc(F)c1

Input SMILES/SMARTS representing molecules to be searched.

構造図

Chemical Draw タブを選択することで構造図の入力フォームを表示する。

Search Forms

Keyword SMILES/SMARTS Chemical Draw

JSME Molecular Editor by Peter Ertl and Bruno Bienfait

Draw and edit molecule structures to be searched.

Query Type: Substructure Query

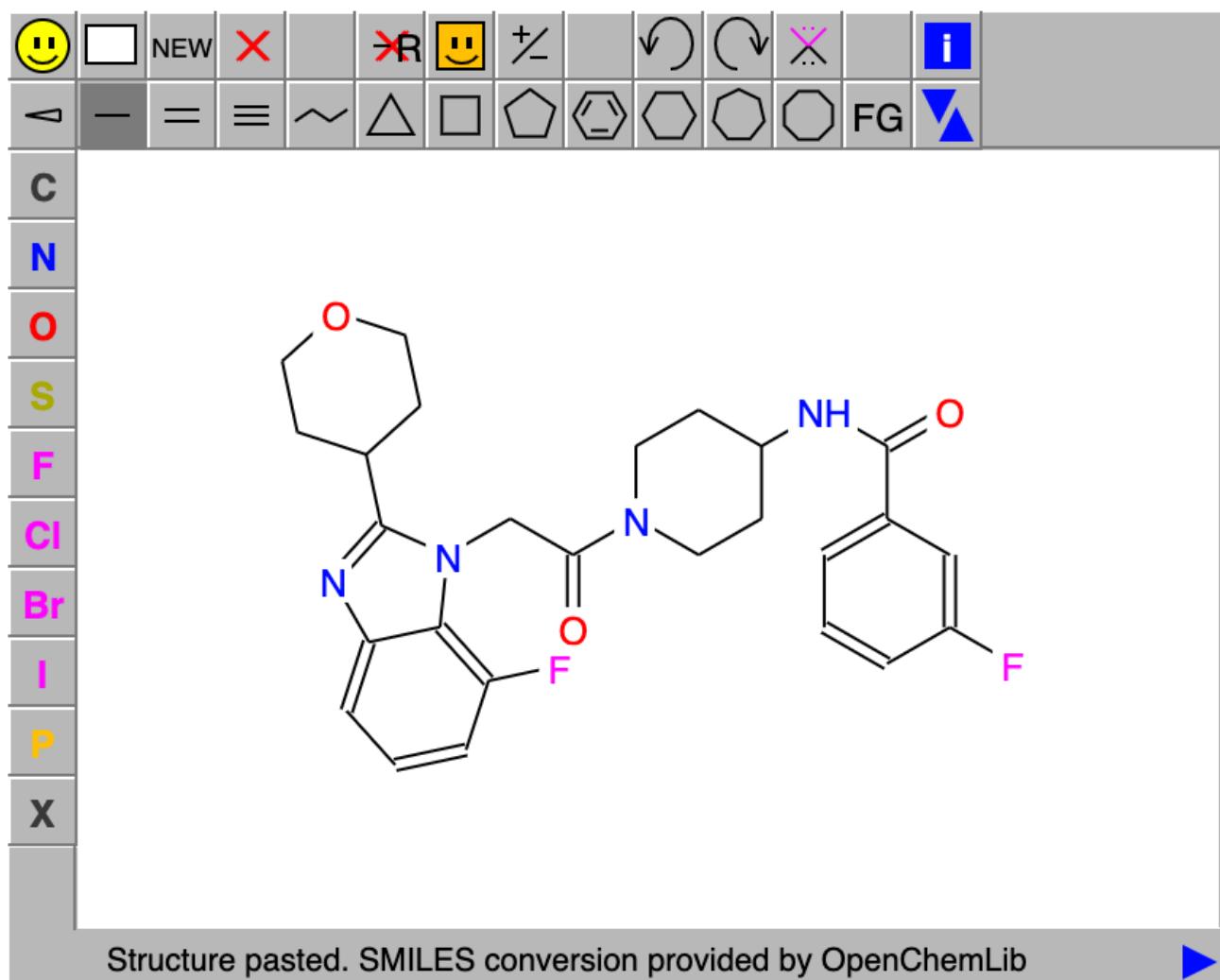
Similarity Threshold: 100%

Advanced Search

Search

The screenshot shows the JSME Molecular Editor interface. At the top, there are three tabs: 'Keyword', 'SMILES/SMARTS' (which is selected), and 'Chemical Draw'. Below these tabs is a toolbar with various chemical drawing and selection tools. To the left of the toolbar is a vertical column of element symbols: C, N, O, S, F, Cl, Br, I, P, and X. The main workspace shows three chemical structures: a cyclopentylamine derivative, a substituted benzimidazole, and a substituted pyrrolidine. Below the workspace, a message states: 'The partial molecule structures appearing most frequently.' At the bottom of the interface, there are dropdown menus for 'Query Type' (set to 'Substructure Query') and 'Similarity Threshold' (set to '100%'), and a 'Search' button.

マウスクリック等の操作により、化合物の構造を描画する。



Draw and edit molecule structures to be searched.

SMILES の読み込み等、Chemical Draw で利用可能な機能については JSME Help and Basic Instructions を参照すること。

キーワード

Keyword タブを選択することで特定のプロパティに対する検索キーワードの入力フォームを表示する。

Search Forms

Keyword SMILES/SMARTS Chemical Draw

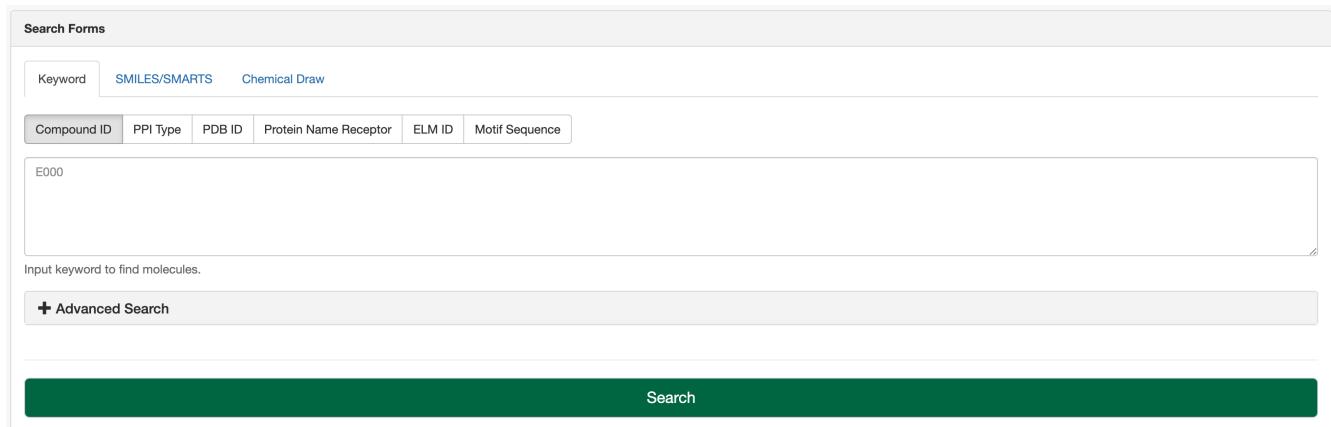
Compound ID PPI Type PDB ID Protein Name Receptor ELM ID Motif Sequence

E000

Input keyword to find molecules.

Advanced Search

Search

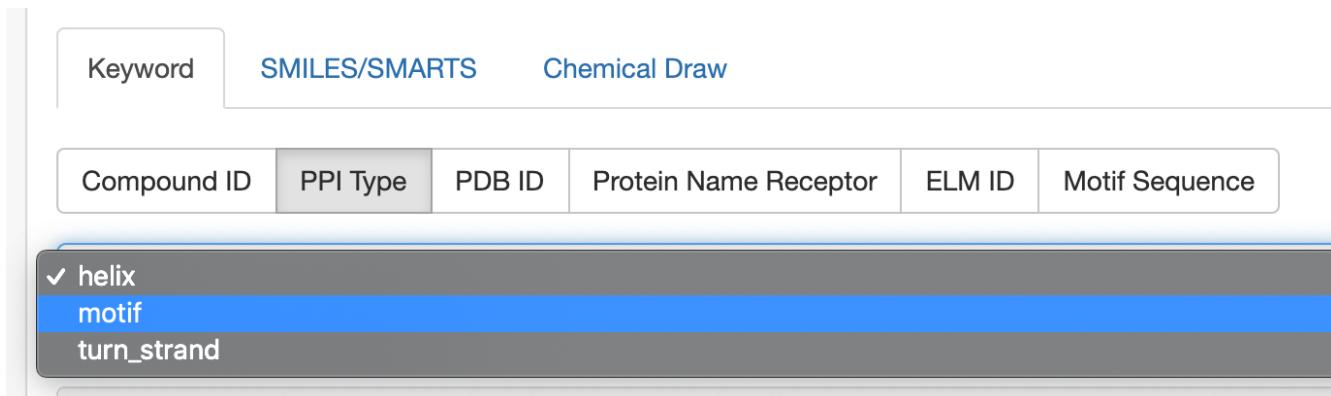


検索対象のプロパティ(PPI Type など)を指定し、キーワードを選択もしくは入力する。

Keyword SMILES/SMARTS Chemical Draw

Compound ID PPI Type PDB ID Protein Name Receptor ELM ID Motif Sequence

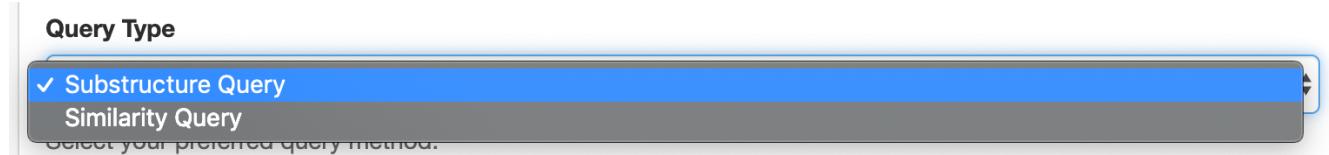
✓ helix
motif
turn_strand



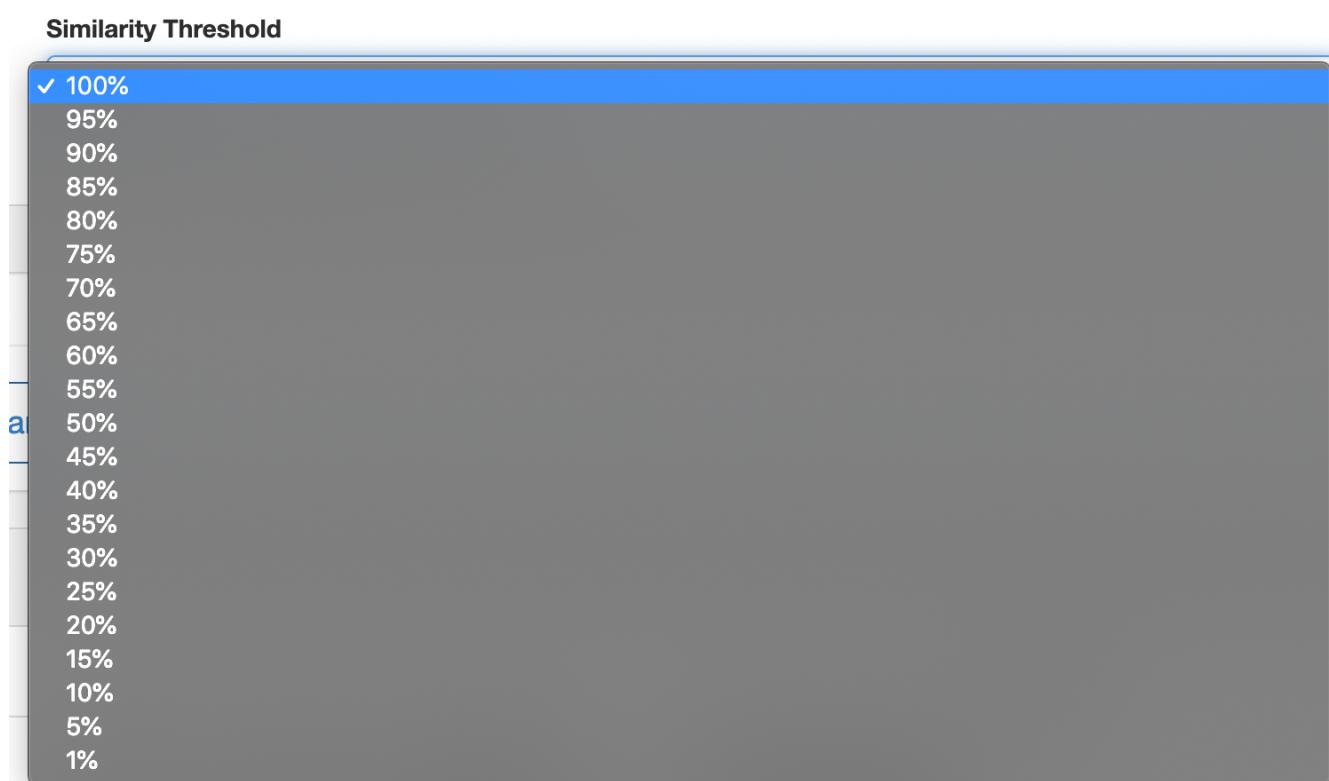
検索方法

構造式または構造図の検索方法は **Query Type** から選択する。

- Substructure Query : 部分一致検索
- Similarity Query : 類似性検索



類似性検索の場合、類似度の閾値(**Similarity Threshold**)を選択する。



数値項目の検索範囲

数値項目の詳細な絞り込みを行う場合は [Advanced Search](#) で値の範囲を指定する。

[Contains NA](#) にチェックを入れることで当該プロパティが設定されていない化合物も検索対象に含めることができる。

Advanced Search

Molecular Weight:	450.0	660.0	<input checked="" type="checkbox"/> Contains NA
MW Monoisotopic:	74.0	4050.0	<input checked="" type="checkbox"/> Contains NA
MolLogP:	-76.0	15.0	<input checked="" type="checkbox"/> Contains NA
XLogP:	-1.0	7.0	<input checked="" type="checkbox"/> Contains NA
Num H Acceptors:	2	14	<input checked="" type="checkbox"/> Contains NA
nHAcceptors:	2	14	<input checked="" type="checkbox"/> Contains NA
HBA:	0	77	<input checked="" type="checkbox"/> Contains NA
HBA Lipinski:	0	107	<input checked="" type="checkbox"/> Contains NA
Num H Donors:	0	6	<input checked="" type="checkbox"/> Contains NA
...			
nAtoms:	26	73	<input checked="" type="checkbox"/> Contains NA
Heavy Atoms:	5	287	<input checked="" type="checkbox"/> Contains NA
QED Weighted:	0.0	1.0	<input checked="" type="checkbox"/> Contains NA
Quantity of Sample mg:	0.0	6247.0	<input checked="" type="checkbox"/> Contains NA
fCsp3:	0.0	1.0	<input checked="" type="checkbox"/> Contains NA
nCarbons:	18	39	<input checked="" type="checkbox"/> Contains NA
nHetAtoms:	4	14	<input checked="" type="checkbox"/> Contains NA
nHalide:	0	5	<input checked="" type="checkbox"/> Contains NA

Search

2.1.2. 検索の実行

検索条件の指定に記載の通り、検索条件を入力した後、Search ボタンを押下する。

Search Forms

Keyword SMILES/SMARTS Chemical Draw

SMILES SMARTS

O=C(NC1CCN(C(=O)Cn2c(C3CCOCC3)nc3cccc(F)c3)CC1)c1cccc(F)c1

Input SMILES/SMARTS representing molecules to be searched.

Query Type Similarity Threshold

Substructure Query 100%
Select your preferred query method. Specify similarity threshold from 1% to 100%.

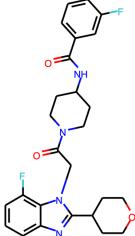
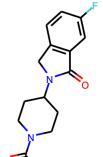
Advanced Search

Search

Search Results に検索条件に合致した化合物の一覧が表示されることを確認する。

Search Results [Column Information](#)

Show 25 entries Showing 1 to 2 of 2 entries [Search:](#)

PPI-ID	Mol Image	MW	XLogP	PPI Type	PDB ID	Receptor Chain	Protein Name Receptor
E000		482.52	3.145	helix	1hqq	1hqq_C	Streptavidin
G1CT		494.53	2.96	motif	4ejc	4ejc_B	Tumor susceptibility gene 101 protein

PROTEIN DATA BANK(PDB)へのアクセス

検索結果に含まれる PDB ID のリンクからPDBの該当ページへアクセスする。

P	PPI Type	PDB ID	Receptor Chain
	helix	1hqq	1hqq_C

RCSB PDB Deposit Search Visualize Analyze Download Learn More MyPDB

PDB 159230 Biological Macromolecular Structures Enabling Breakthroughs in Research and Education

Search by PDB ID, author, macromolecule, sequence, or ligands Go Advanced Search | Browse by Annotations

PDB-101 Worldwide Protein Data Bank EMDataResource Protein Data Bank Foundation Nucleic Acid Database

Structure Summary 3D View Annotations Sequence Sequence Similarity Structure Similarity Experiment

1HQQ

MINIPROTEIN MP-2 (M9A) COMPLEX WITH STREPTAVIDIN

DOI: 10.2210/pdb1HQQ/pdb

Classification: UNKNOWN FUNCTION

Organism(s): *Streptomyces avidinii*

Expression System: *Escherichia coli*

Deposited: 2000-12-19 Released: 2003-09-16

Deposition Author(s): [Yang, H.W., Liu, D.Q., Fan, X., White, M.A., Fox, R.O.](#)

Experimental Data Snapshot

Method: X-RAY DIFFRACTION Resolution: 1.7 Å R-Value Free: 0.249 R-Value Work: 0.224

wwPDB Validation

Metric	Percentile Ranks	Value
Rfree	6	0.250
Clashscore	10	6
Ramachandran outliers	1.5%	1.5%
Sidechain outliers	13.4%	13.4%
RSRZ outliers	Worse	Better

This is version 1.2 of the entry. See complete [history](#).

Literature Download Primary Citation

Conformational Ensemble Analysis of Ligand Binding in Streptavidin Mini-protein

ELMへのアクセス

検索結果に含まれる **ELM ID** のリンクからELMの該当ページへアクセスする。

ELM ID
DEG_SIAH_1

ELM The Eukaryotic Linear Motif resource for Functional Sites in Proteins

Search ELM Database

ELM Home ELM Prediction ELM DB ELM Candidates ELM Information ELM downloads Help

«[DEG_SCF_TRCP1_1](#)» [»DEG_SPOP_SBC_1»](#)

DEG_SIAH_1

Accession: [ELME000241](#)

Functional site class: Siah binding Motif

Functional site description: The members of the SINA/Siah family have domain architecture consisting of a RING domain, two zinc finger motifs and a substrate/adaptor binding domain (SBD) that mediates the interaction with the binding partners.

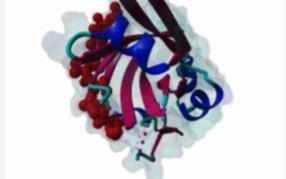
ELM Description: The PxAxVxP motif was first described to confer a high-affinity binding to the Siah/PHYL interaction. It has been detected in other Siah interacting proteins, including DCC, KLF10, OBF-1. The motif binds by partial Beta-augmentation. The present pattern is stricter than proposed by [House,2006](#). It will find most verified instances but may miss some candidates.

Pattern: [.P.A.V.P\[^P\]](#)

Pattern Probability: 0.0000271

Present in taxon:  Metazoa

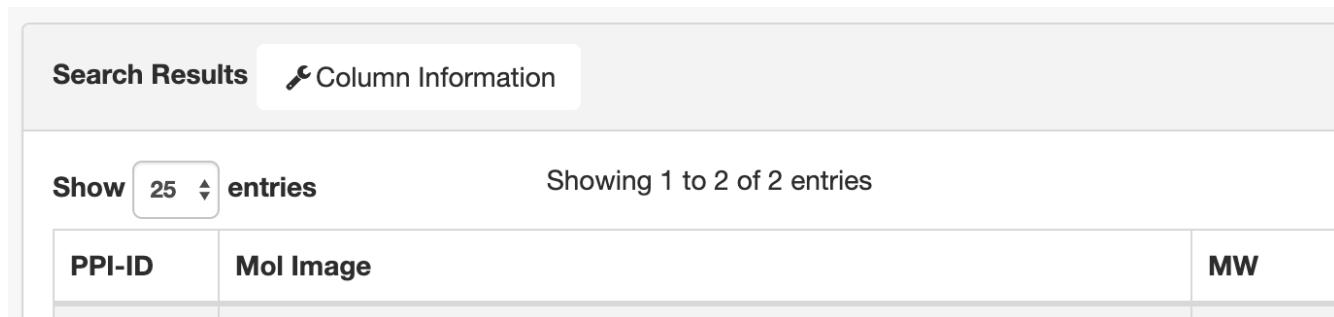
Interaction Domain:  Sina (PF03145) Seven in absentia protein family (Stoichiometry: 1 : 1)

PDB Structure:  2A25 

■ See 9 Instances for DEG_SIAH_1

表示カラムの指定

カラムの説明を確認する場合や、表示・非表示を切り替える場合は **Column Information** を押下する。

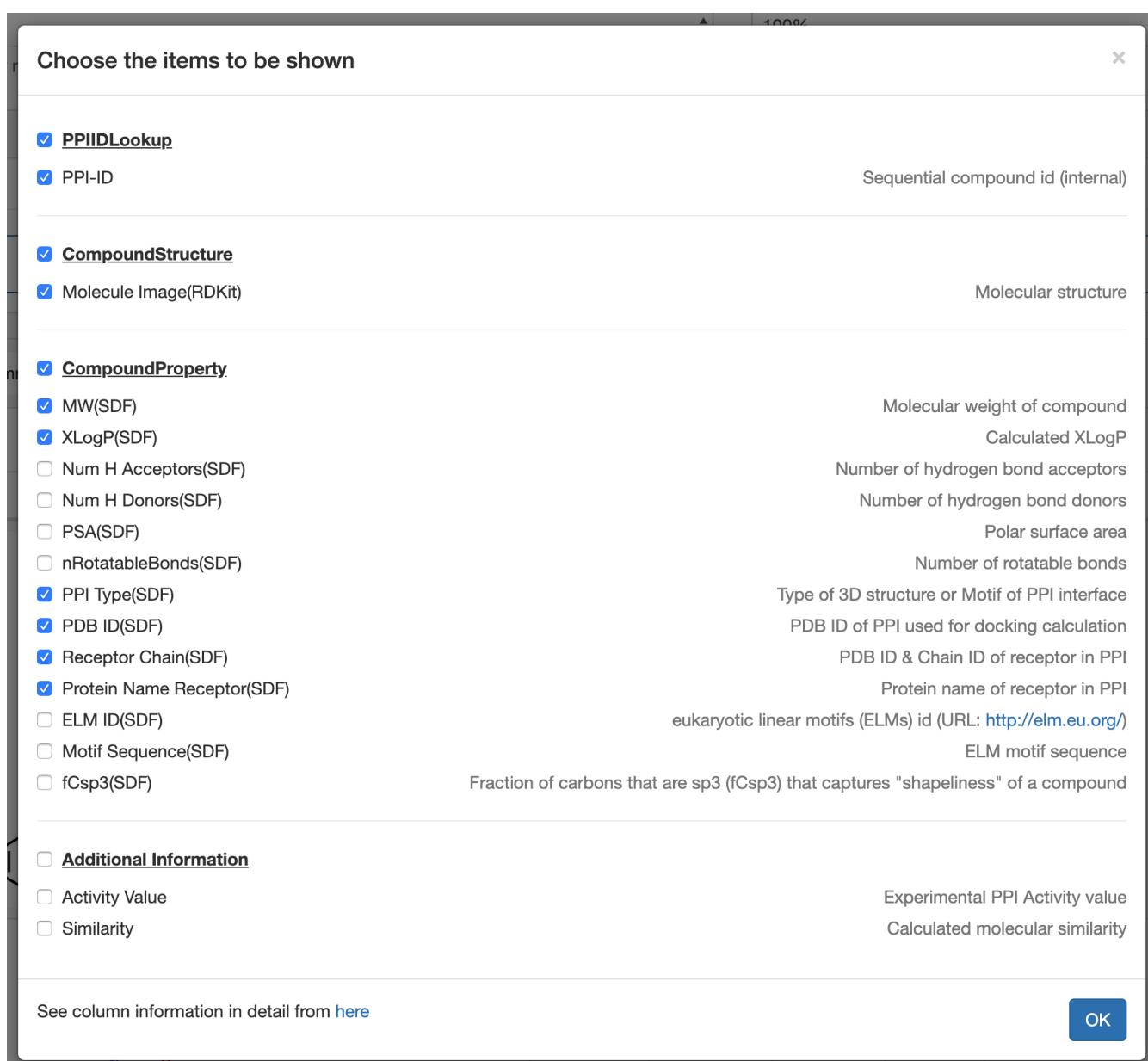


Search Results Column Information

Show 25 entries Showing 1 to 2 of 2 entries

PPI-ID	Mol Image	MW

カラムごとのチェックボックスで表示・非表示を切り替えることができる。



Choose the items to be shown

<input checked="" type="checkbox"/> <u>PPIIDLookup</u>	Sequential compound id (internal)
<input checked="" type="checkbox"/> PPI-ID	
<input checked="" type="checkbox"/> <u>CompoundStructure</u>	Molecular structure
<input checked="" type="checkbox"/> Molecule Image(RDKit)	
<input checked="" type="checkbox"/> <u>CompoundProperty</u>	Molecular weight of compound
<input checked="" type="checkbox"/> MW(SDF)	Calculated XLogP
<input checked="" type="checkbox"/> XLogP(SDF)	
<input type="checkbox"/> Num H Acceptors(SDF)	Number of hydrogen bond acceptors
<input type="checkbox"/> Num H Donors(SDF)	Number of hydrogen bond donors
<input type="checkbox"/> PSA(SDF)	Polar surface area
<input type="checkbox"/> nRotatableBonds(SDF)	Number of rotatable bonds
<input checked="" type="checkbox"/> PPI Type(SDF)	Type of 3D structure or Motif of PPI interface
<input checked="" type="checkbox"/> PDB ID(SDF)	PDB ID of PPI used for docking calculation
<input checked="" type="checkbox"/> Receptor Chain(SDF)	PDB ID & Chain ID of receptor in PPI
<input checked="" type="checkbox"/> Protein Name Receptor(SDF)	Protein name of receptor in PPI
<input type="checkbox"/> ELM ID(SDF)	eukaryotic linear motifs (ELMs) id (URL: http://elm.eu.org/)
<input type="checkbox"/> Motif Sequence(SDF)	ELM motif sequence
<input type="checkbox"/> fCsp3(SDF)	Fraction of carbons that are sp3 (fCsp3) that captures "shapeliness" of a compound
<input type="checkbox"/> <u>Additional Information</u>	
<input type="checkbox"/> Activity Value	Experimental PPI Activity value
<input type="checkbox"/> Similarity	Calculated molecular similarity

See column information in detail from [here](#) OK

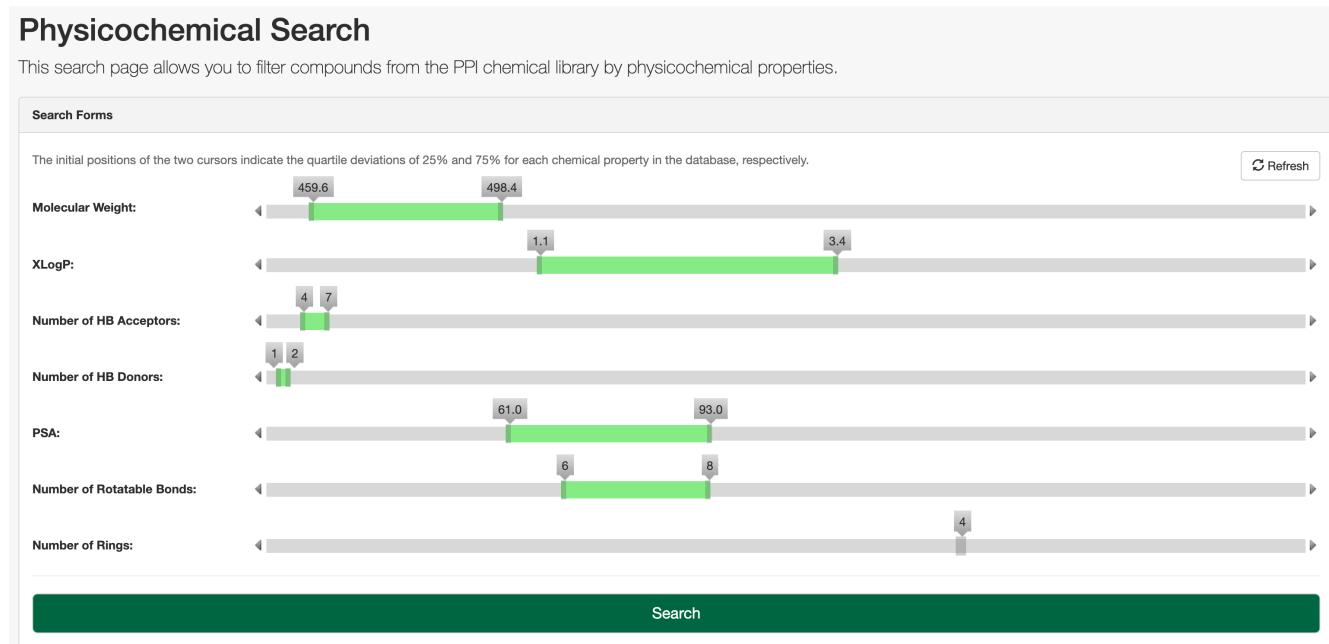
3. Advanced Search

3.1. Physicochemical Search

サイドメニューの **Physicochemical** またはトップページの **Physicochemical Search** からアクセスする。

検索条件は**数値項目の検索範囲**と同様にスライダーで指定することができる。

検索結果の表示内容については**PPI Library Search**を参照すること。



3.2. Druglikeness Search

サイドメニューの **Druglikeness** またはトップページの **Druglikeness Search** からアクセスする。

検索条件は**数値項目の検索範囲**と同様のスライダーやチェックボックスで指定することができる。

検索結果の表示内容については**PPI Library Search**を参照すること。

Druglikeness Search

This search page allows you to filter compound structures from the PPI library by drug-likeness indices (Lipinski's Rule of 5, the QED drug-likeness score, a fraction of sp3 carbon atoms) and solubility.

Search Forms

Num Lipinski RO5 Violations:  Refresh

QED Weighted:  0.5 1.0

fCsp3:  0.5 1.0

Solubility: Moderately Highly Very Soluble Poorly Insoluble

PPI Type: Helix Motif Turn Strand

Search

4. Curation Search

4.1. Compound Search

サイドメニューの **CURATION SEARCH > Compound Search** またはトップページの **Curation Data Compound Search** からアクセスする。

検索方法については **PPI Library Search** と同様であるが、以下の点のみ異なる。

- キーワード検索は行えない。
- Advanced Search** では下図の項目のみ検索することができる。また、**PPI Activity** でPPIの活性・非活性（実験値）を指定することができる。

Advanced Search

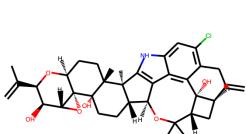
Molecular Weight:	74.0	4050.0	<input checked="" type="checkbox"/> Contains NA
MW Monoisotopic:	74.0	4050.0	<input checked="" type="checkbox"/> Contains NA
XLogP:	-35.0	18.0	<input checked="" type="checkbox"/> Contains NA
MolLogP:	-76.0	15.0	<input checked="" type="checkbox"/> Contains NA
HBA:	0	77	<input checked="" type="checkbox"/> Contains NA
HBA Lipinski:	0	107	<input checked="" type="checkbox"/> Contains NA
HBD:	0	61	<input checked="" type="checkbox"/> Contains NA
HBD Lipinski:	0	71	<input checked="" type="checkbox"/> Contains NA
PSA:	0.0	1763.0	<input checked="" type="checkbox"/> Contains NA
Number of Rotatable Bonds:	0	132	<input checked="" type="checkbox"/> Contains NA
Number of Rings:	0	13	<input checked="" type="checkbox"/> Contains NA
Aromatic Rings:	0	10	<input checked="" type="checkbox"/> Contains NA
Heavy Atoms:	5	287	<input checked="" type="checkbox"/> Contains NA
QED Weighted:	0.0	1.0	<input checked="" type="checkbox"/> Contains NA
PPI Activity:	<input checked="" type="checkbox"/> Active		
	<input checked="" type="checkbox"/> Inactive		

- 検索結果で表示するカラムは下図の通りである。Active にはPPIの実験値が活性状態であった場合にチェックマークを表示する。

Search Results 

Showing 1 to 25 of 1,567 entries

Search:

PPI-ID	Mol Image	MW	XLogP	HBA	HBD	PSA	nRotatableBonds	nRings	Common Target Pref Name	Active
J3Q2		634.213	3.369	6	4	107.47	1	10	Runt-related transcription factor 1/Core-binding factor subunit beta	
D530		696.858	-1.206	12	4	145.76	3	12	HIF-1a/p300	

Choose the items to be shown

PPIIDLookup Sequential compound id (internal)

PPI-ID

CompoundStructure Molecular structure

Mol Image(RDKit)

CompoundProperty

MW(RDKit) Molecular weight of compound

MW Monoisotopic(RDKit) Monoisotopic parent molecular weight

XLogP(CDK) Calculated XLogP

MolLogP(RDKit) Calculated MolLogP

HBA(RDKit) Number of hydrogen bond acceptors

HBA Lipinski(RDKit) Number of hydrogen bond acceptors calculated according to Lipinski's original rules (i.e., N + O count)

HBD(RDKit) Number of hydrogen bond donors

HBD Lipinski(RDKit) Number of hydrogen bond donors calculated according to Lipinski's original rules (i.e., NH + OH count)

PSA(RDKit) Polar surface area

nRotatableBonds(RDKit) Number of rotatable bonds

nRings(RDKit) Number of ring systems

Aromatic Rings(RDKit) Number of aromatic rings

Heavy Atoms(RDKit) Number of heavy (non-hydrogen) atoms

QED Weighted(RDKit) Weighted quantitative estimate of drug likeness (as defined by Bickerton et al., Nature Chem 2012)

Target Pref Name Target preferred name(Uniprot)

Common Target Pref Name Common target preferred name(Uniprot)

Additional Information

Active Experimental PPI Activity

Activity Value Experimental PPI Activity value

Similarity Calculated molecular similarity

See column information in detail from [here](#)

4.2. Target Search

サイドメニューの **CURATION SEARCH > Target Search** またはトップページの **Curation Data Target Search** からアクセスする。

Compound Searchと以下の点のみ異なる。

- キーワード検索では **Common Target Pref Name** の選択、もしくは **Target Pref Name** の部分一致検索を行うことができる。

Search Forms

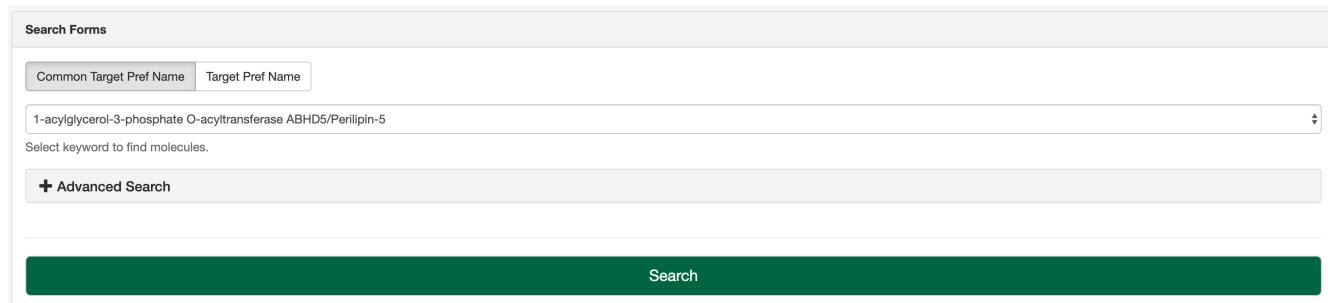
Common Target Pref Name Target Pref Name

1-acylglycerol-3-phosphate O-acyltransferase ABHD5/Perilipin-5

Select keyword to find molecules.

Advanced Search

Search



- Advanced Search** では下図の項目のみ検索することができる。下図右上のボタンを押下することで **Rule of 5**、**Rule of 4 for PPI**、**Beyond Rule of 5** および **All** (全件検索)の検索条件を適用することができる。

Advanced Search

Rule of 5 Rule of 4 for PPI Beyond Rule of 5 All

検索項目	範囲	値	条件
Molecular Weight:	74.0 - 500.0		<input checked="" type="checkbox"/> Contains NA
XLogP:	-35.0 - 5.0		<input checked="" type="checkbox"/> Contains NA
HBA:	0 - 10		<input checked="" type="checkbox"/> Contains NA
HBD:	0 - 5		<input checked="" type="checkbox"/> Contains NA
PSA:	0.0 - 1763.0		<input checked="" type="checkbox"/> Contains NA
Number of Rotatable Bonds:	0 - 132		<input checked="" type="checkbox"/> Contains NA
Number of Rings:	0 - 13		<input checked="" type="checkbox"/> Contains NA
PPI Activity:			

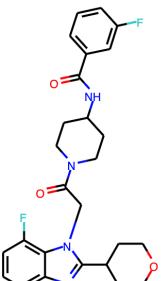


5. Compound Information

化合物検索結果の **PPI-ID** をクリックすることで化合物ごとの個別ページに遷移する。

Search Results 

Show 25 entries Showing 1 to 2 of 2 entries

PPI-ID	Mol Image	MW	XLogP
E000		482.52	3.145

化合物個別画面では選択した化合物の詳細情報を確認することができる。

DLIP

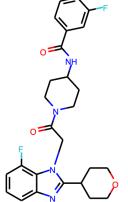
PPI LIBRARY SEARCH
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ADVANCED SEARCH
○ Physicochemical
○ Druglikeness

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Compound Information

Item	Value
KLNUMBER(SDF)	KL-001-1269-864
Mol Image(RDKit)	
Standard Inchi(RDKit)	InChI=1S/C26H28F2N4O3/c27-19-4-1-3-18(15-19)26(34)29-20-7-11-31(12-8-20)23(33)16-32-24-21(28)5-2-6-22(24)30-25(32)17-9-13-35-14-10-17/h1-6,15,17,20H,7-14,16H2,(H,29,34)
Standard Inchi Key(RDKit)	RXEYMFNLNNJIOFZ-UHFFFAOYSA-N
Canonical SMILES(RDKit)	O=[N+]1CCN(C(=O)Cc2c(C3CCOCC3)nc3cccc(F)c3)CC1c1ccccc(F)c1
SMILES(SDF)	c1cc(cc(c1)F)C(=O)NC2CCN(CC2)C(=O)Cc3c4cccc4F)nc3C5CCOCC5
MW(SDF)	482.52
MW(RDKit)	482.531
MW Monoisotopic(RDKit)	482.212947196
MolLogP(RDKit)	3.6295
XLogP(SDF)	3.145
XLogP(CDK)	3.269
Num H Acceptors(SDF)	7
nHAcceptors(SDF)	7
HBA(RDKit)	5
HBA Lipinski(RDKit)	7

6. About

6.1. About DB

サイドメニューの [About > About DB](#) からアクセスする。

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About DB

About PPI Library

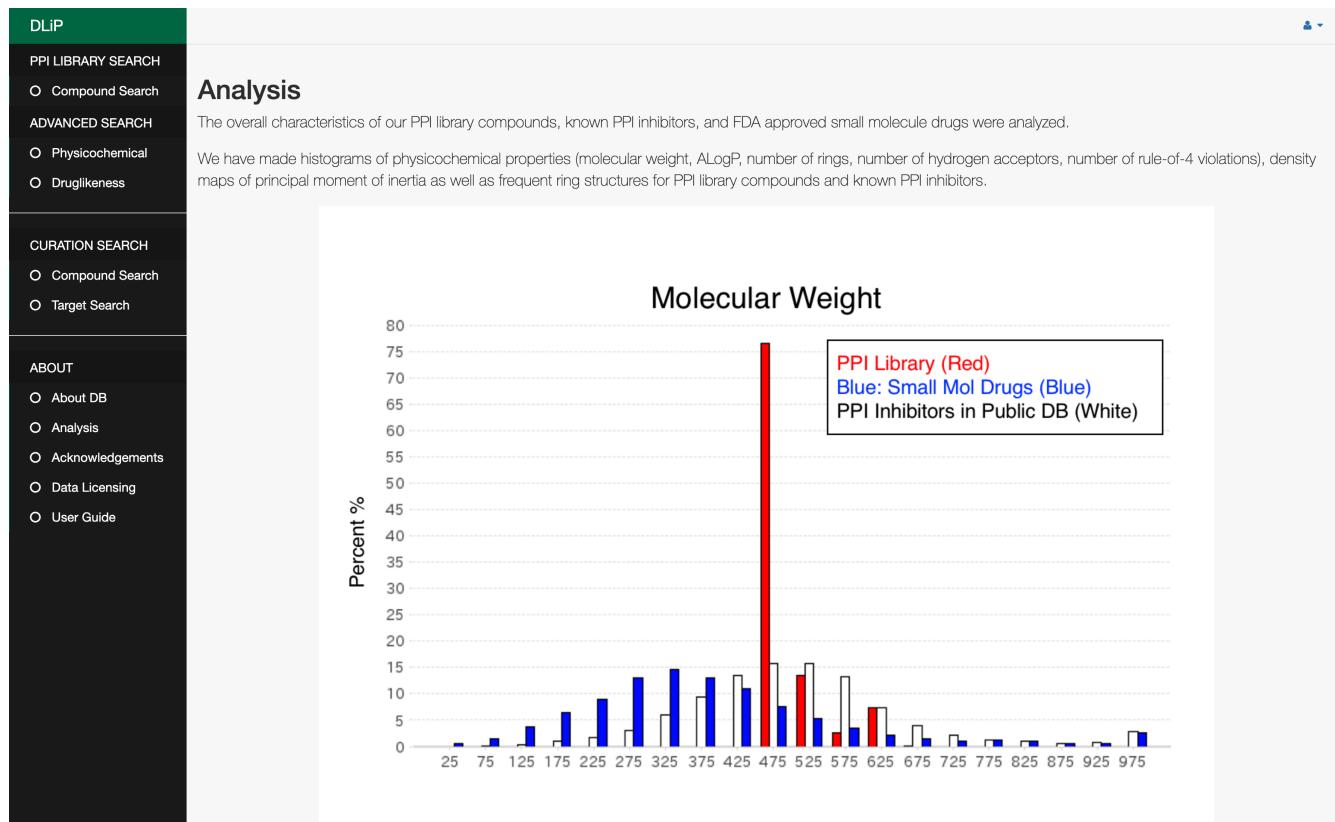
This database contains 15,000 compounds expected to PPI inhibitions and selected from a virtual compound library (K-Library developed by Kishida Chemical Co, Ltd., ~8M compounds). We conducted docking calculation against the virtual library on PDB structures of known PPI targets. Then, we selected and synthesized about 100 compounds from each target. Furthermore, our PPI library also includes novel compounds with new scaffolds and unique 3D shapes (sphere-like structures). Thus, our PPI library is useful for medium-sized drug discovery.

About Database

This database has been developed by Keio University and PeptiDream Inc. During this development, NIBIOHN supports and advises this project. This work is supported by AMED (Japan Agency for Medical Research and Development) grant.

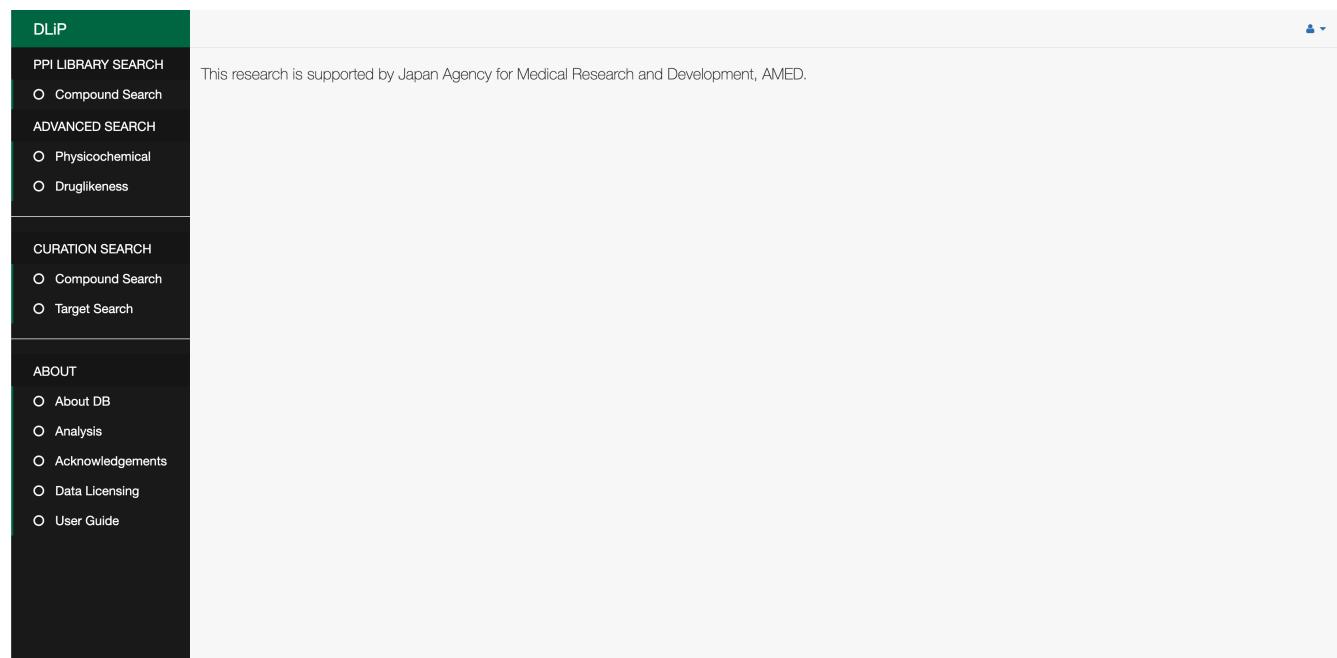
6.2. Analysis

サイドメニューの **About > Analysis** からアクセスする。



6.3. Acknowledgements

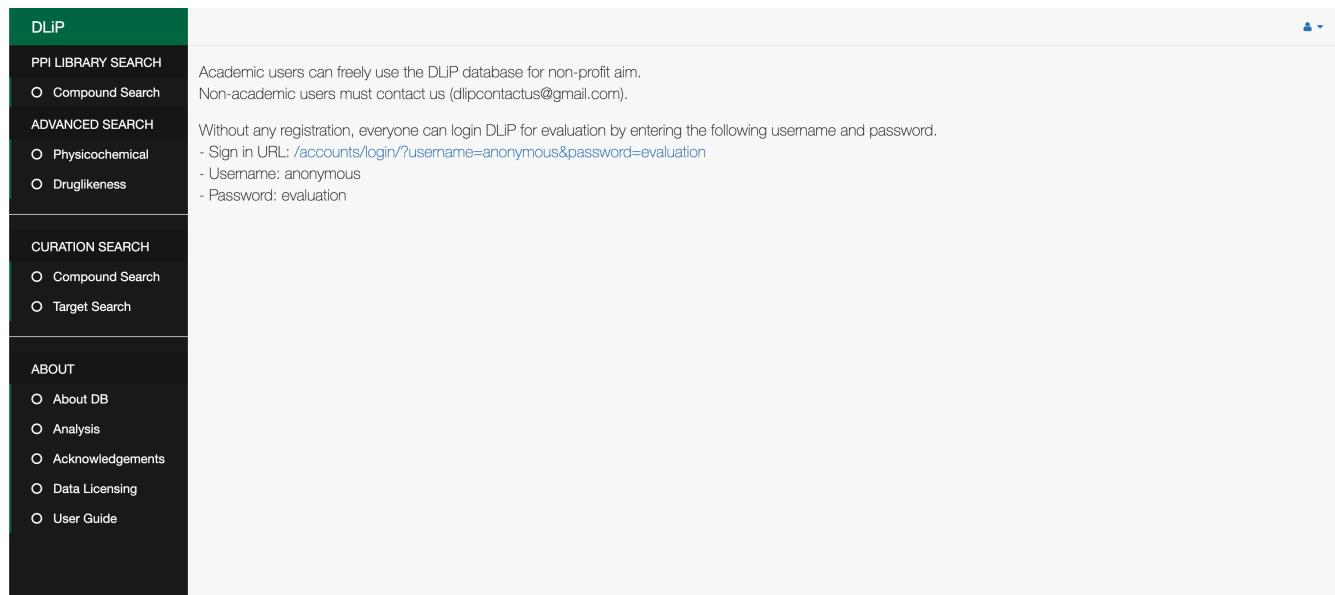
サイドメニューの [About > Acknowledgements](#) からアクセスする。



The screenshot shows the DLiP interface with a dark sidebar on the left and a light content area on the right. The sidebar contains three main sections: 'PPI LIBRARY SEARCH', 'CURATION SEARCH', and 'ABOUT'. The 'ABOUT' section is currently selected and expanded, showing links for 'About DB', 'Analysis', 'Acknowledgements', 'Data Licensing', and 'User Guide'. The main content area on the right displays a single line of text: 'This research is supported by Japan Agency for Medical Research and Development, AMED.' There is also a small user icon in the top right corner of the content area.

6.4. Data Licensing

サイドメニューの **About > Data Licensing** からアクセスする。



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Academic users can freely use the DLiP database for non-profit aim.
Non-academic users must contact us (dlipcontactus@gmail.com).

Without any registration, everyone can login DLiP for evaluation by entering the following username and password.

- Sign in URL: [/accounts/login/?username=anonymous&password=evaluation](#)
- Username: anonymous
- Password: evaluation

6.5. User Guide

サイドメニューの [About > User Guide](#) からアクセスする。

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Column Information

Column Name	Description	
PPI-ID	Unique compound id (internal) The information source of compounds can be identified by an initial character of PPI-ID. K: IPPI-DB A: 2P2I-DB D: TIMBAL J: ChEMBL B: Journal of Medical Chemistry C, E, F, G, H, and I: newly synthesized in DLIP	
Compound Property	Molecular Weight	Molecular weight of compound
	MW Monoisotopic	Monoisotopic parent molecular weight
	MolLogP	Calculated MolLogP
	XLogP	Calculated XLogP
	Num H Acceptors/HBA	Number of hydrogen bond acceptors
	HBA Lipinski	Number of hydrogen bond acceptors calculated according to Lipinski's original rules (i.e., N + O count)
	Num H Donors/HBD	Number of hydrogen bond donors
	HBD Lipinski	Number of hydrogen bond donors calculated according to Lipinski's original rules (i.e., NH + OH count)
	PSA	Polar surface area
	nRotatableBonds	Number of rotatable bonds
	nRings	Number of ring systems
	Aromatic Rings	Number of aromatic rings
Heavy Atoms	Number of heavy (non-hydrogen) atoms	
QED Weighted	Weighted quantitative estimate of druglikeness (as defined by Bickerton et al., Nature Chem 2012)	
PPI Chemical Library Feature	PPI Type	Type of 3D structure or Motif of PPI interface
	PDB ID	PDB ID of PPI used for docking calculation
	Receptor Chain	PDB ID & Chain ID of receptor in PPI

7. ログアウト

画面右上のメニューからLogoutを押下することでログアウトする。

