

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

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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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。

DLIP

Please Sign In

Username

Password

Login

Free for non-commercial academic use | [Learn more](#)

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: 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。

Search Forms

Keyword

SMILES/SMARTS

Chemical Draw

SMILES

SMARTS

Input SMILES/SMARTS representing molecules to be searched.

Query Type

Substructure Query

Similarity Threshold

100%

Select your preferred query method.

Specify similarity threshold from 1% to 100%.

+ Advanced Search

Search

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

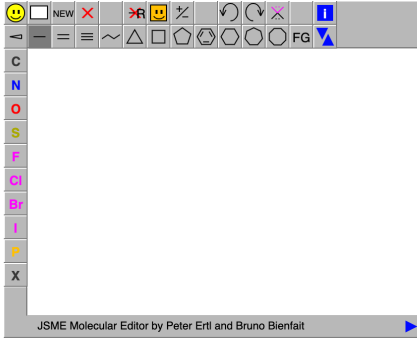
Input SMILES/SMARTS representing molecules to be searched.

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

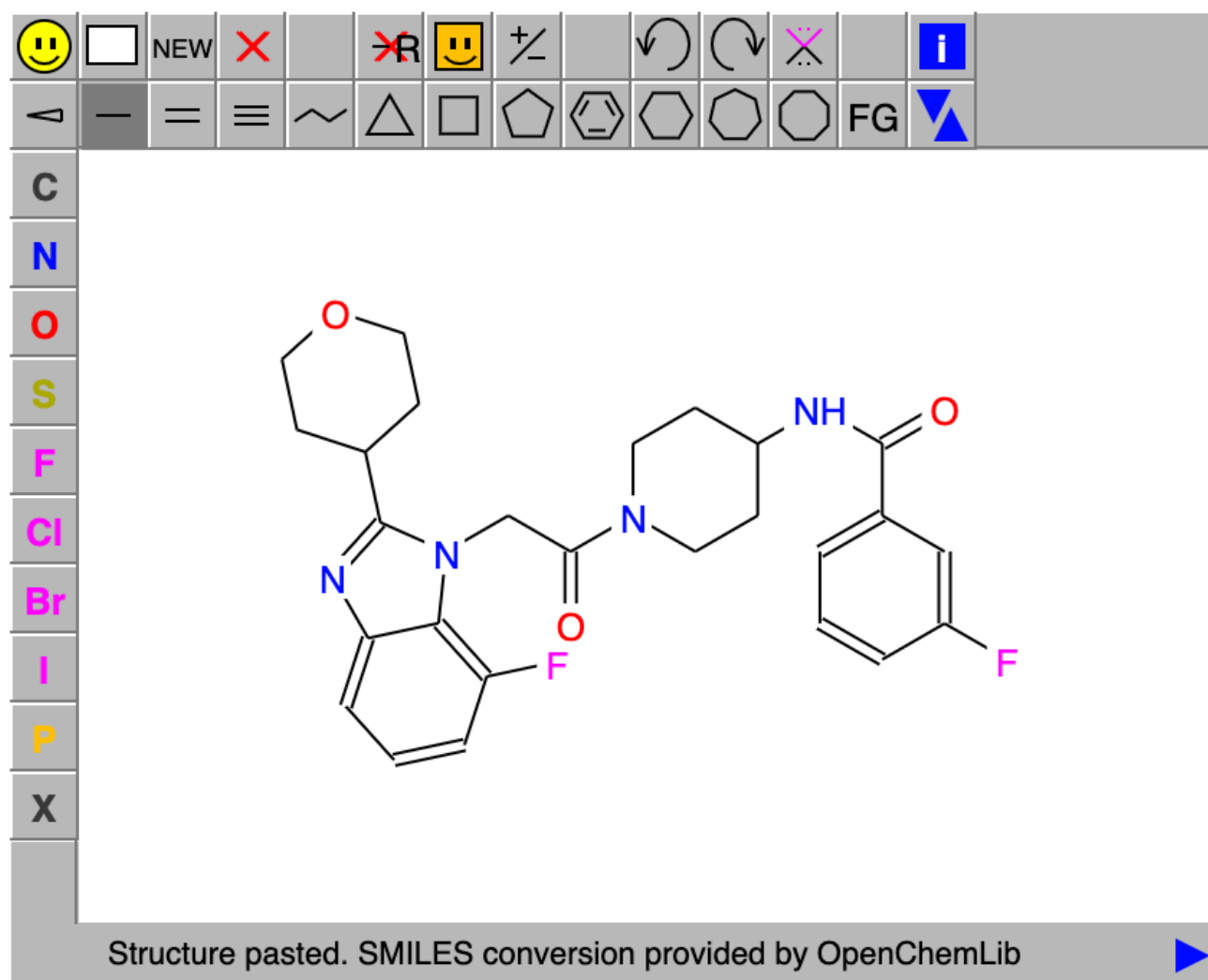
Substructure Query

Select your preferred query method.

+ Advanced Search

Search

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

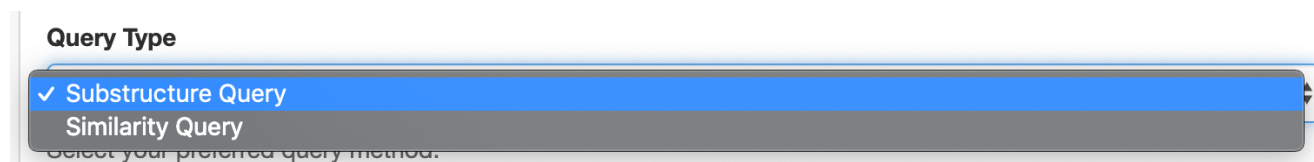
motif

turn_strand

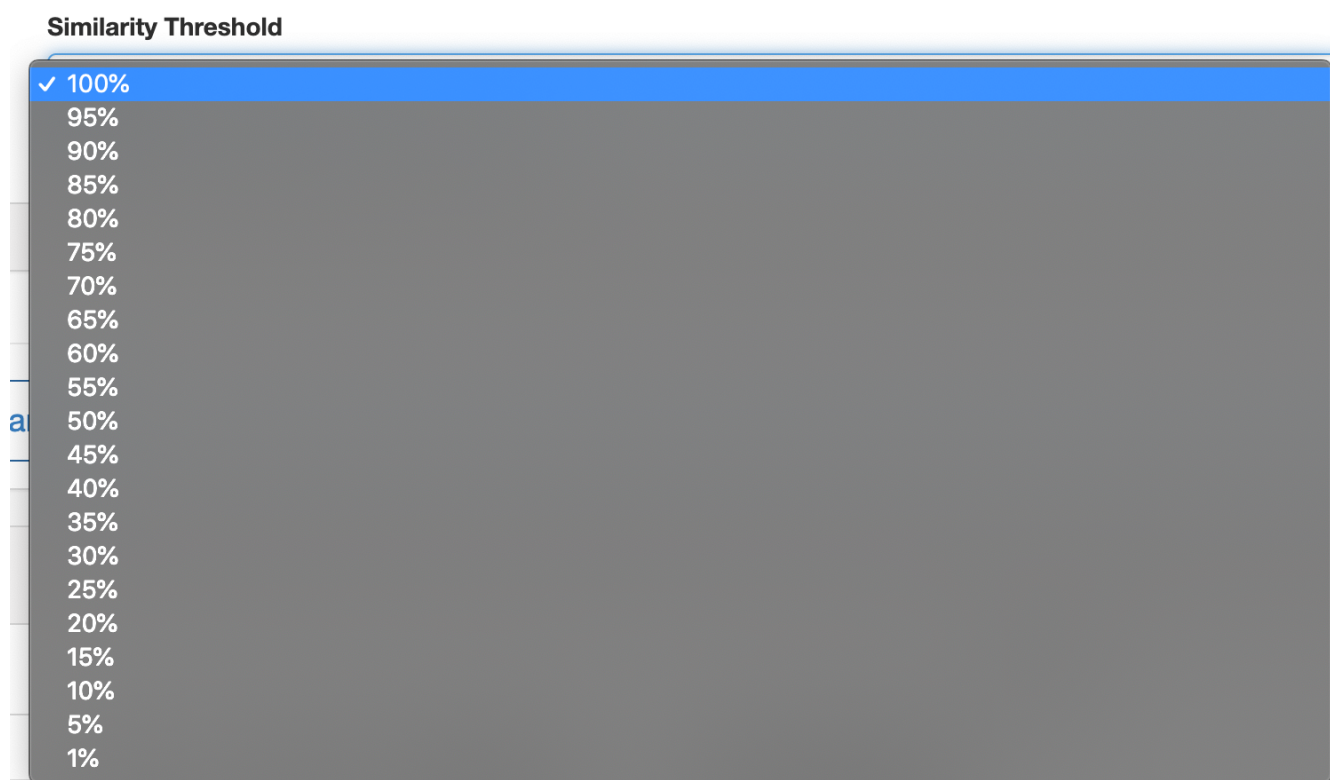
検索方法

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:

450.0660.0

☒ Contains NA

MW Monoisotopic:

74.04050.0

☒ Contains NA

MolLogP:

-76.015.0

☒ Contains NA

XLogP:

-1.07.0

☒ Contains NA

Num H Acceptors:

214

☒ Contains NA

nHAcceptors:

214

☒ Contains NA

HBA:

077

☒ Contains NA

HBA Lipinski:

0107

☒ Contains NA

Num H Donors:

06

☒ Contains NA

...

nAtoms:

2673

☒ Contains NA

Heavy Atoms:

5287

☒ Contains NA

QED Weighted:

0.01.0

☒ Contains NA

Quantity of Sample mg:

0.06247.0

☒ Contains NA

fCsp3:

0.01.0

☒ Contains NA

nCarbons:

1839

☒ Contains NA

nHetAtoms:

414

☒ Contains NA

nHalide:

05

☒ 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)c32)CC1)c1cccc(F)c1

Input SMILES/SMARTS representing molecules to be searched.

Query Type

Substructure Query

Select your preferred query method.

Similarity Threshold

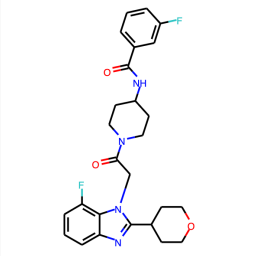
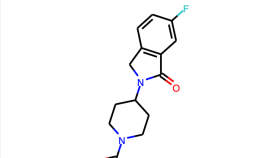
100%

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: <input type="text"/>					
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	4eje	4eje_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

RCSB PDB

PROTEIN DATA BANK

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 PDB PROTEIN DATA BANK

EMDataResource Unified Data Resource for 3DSD

NUCLEIC ACID DATABASE

Worldwide Protein Data Bank Foundation

Facebook

Twitter

YouTube

LinkedIn

Structure Summary

3D View

Annotations

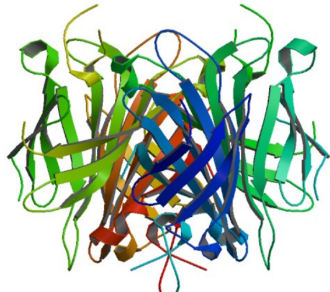
Sequence

Sequence Similarity

Structure Similarity

Experiment

Biological Assembly 1 ?



3D View: Structure | Electron Density

Standalone Viewers

[Protein Workshop](#) | [Ligand Explorer](#)

Global Symmetry: Dihedral - D2 (3D View)

Global Stoichiometry: Homo 4-mer - A4

Biological assembly 1 assigned by authors and generated by PISA (software)

1HQQ

MINIPROTEIN MP-2 (M9A) COMPLEX WITH STREPTAVIDIN

DOI: [10.2210/pdb1HQQ/pdb](https://doi.org/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

3D Report

Full Report

Metric	Percentile Ranks	Value
Rfree		0.250
Clashscore		6
Ramachandran outliers		0
Sidechain outliers		1.5%
RSRZ outliers		13.4%

Worse

Better

■ Percentile relative to all X-ray structures

□ Percentile relative to X-ray structures of similar resolution

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



The Eukaryotic Linear Motif resource for
Functional Sites in Proteins

[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 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 ×

☒ **PPIIDLookup**

☒ PPI-ID Sequential compound id (internal)

☒ **CompoundStructure**

☒ Molecule Image(RDKit) Molecular structure

☒ **CompoundProperty**

☒ MW(SDF) Molecular weight of compound

☒ XLogP(SDF) Calculated XLogP

☐ Num H Acceptors(SDF) Number of hydrogen bond acceptors

☐ Num H Donors(SDF) Number of hydrogen bond donors

☐ PSA(SDF) Polar surface area

☐ nRotatableBonds(SDF) Number of rotatable bonds

☒ PPI Type(SDF) Type of 3D structure or Motif of PPI interface

☒ PDB ID(SDF) PDB ID of PPI used for docking calculation

☒ Receptor Chain(SDF) PDB ID & Chain ID of receptor in PPI

☒ Protein Name Receptor(SDF) Protein name of receptor in PPI

☐ ELM ID(SDF) eukaryotic linear motifs (ELMs) id (URL: <http://elm.eu.org/>)

☐ Motif Sequence(SDF) ELM motif sequence

☐ fCsp3(SDF) Fraction of carbons that are sp3 (fCsp3) that captures "shapeliness" of a compound

☐ **Additional Information**

☐ Activity Value Experimental PPI Activity value

☐ 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。

Physicochemical Search

This search page allows you to filter compounds from the PPI chemical library by physicochemical properties.

Search Forms

The initial positions of the two cursors indicate the quartile deviations of 25% and 75% for each chemical property in the database, respectively. Refresh

Molecular Weight:

459.6

498.4

XLogP:

1.1

3.4

Number of HB Acceptors:

4

7

Number of HB Donors:

1

2

PSA:

61.0

93.0

Number of Rotatable Bonds:

6

8

Number of Rings:

4

Search

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: 0

QED Weighted: 0.5 1.0

fCsp3: 0.5 1.0

Solubility: ☒ Moderately ☒ Highly ☒ Very ☒ Soluble ☐ Poorly ☐ Insoluble

PPI Type: ☒ Helix ☒ Motif ☒ Turn Strand

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

Contains NA

MW Monoisotopic:

74.0

4050.0

Contains NA

XLogP:

-35.0

18.0

Contains NA

MolLogP:

-76.0

15.0

Contains NA

HBA:

0

77

Contains NA

HBA Lipinski:

0

107

Contains NA

HBD:

0

61

Contains NA

HBD Lipinski:

0

71

Contains NA

PSA:

0.0

1763.0

Contains NA

Number of Rotatable Bonds:

0

132

Contains NA

Number of Rings:

0

13

Contains NA

Aromatic Rings:

0

10

Contains NA

Heavy Atoms:

5

287

Contains NA

QED Weighted:

0.0

1.0


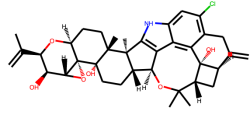

Contains NA

PPI Activity:

Active

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 											
Show 25 entries		Showing 1 to 25 of 1,567 entries								Search: <input type="text"/>	
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		
D53O		696.858	-1.206	12	4	145.76	3	12	HIF-1a/p300		✓

Choose the items to be shown

☒ **PPIIDLookup**

☒ PPI-ID

Sequential compound id (internal)

☒ **CompoundStructure**

☒ Mol Image(RDKit)

Molecular structure

☒ **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](#)

OK

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

Molecular Weight:

74.0500.0

Contains NA

XLogP:

-35.05.0

Contains NA

HBA:

010

Contains NA

HBD:

05

Contains NA

PSA:

0.01763.0

Contains NA

Number of Rotatable Bonds:

0132

Contains NA

Number of Rings:

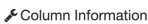
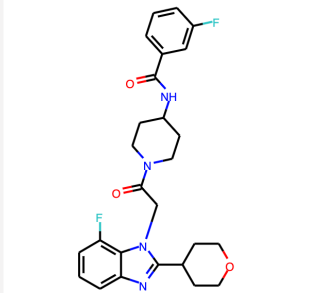
013

Contains NA

PPI Activity:

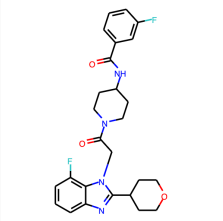
5. Compound Information

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	
○ Compound Search	
ADVANCED SEARCH	
○ Physicochemical	
○ Druglikeness	
CURATION SEARCH	
○ Compound Search	
○ Target Search	
ABOUT	
○ About DB	
○ Analysis	
○ Acknowledgements	
○ Data Licensing	
○ User Guide	

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)	RXEYMLNINJOFZ-UHFFFAOYSA-N
Canonical SMILES(RDKit)	O=C([N]1CCN(C(=O)Cn2c(C3CCOCC3)nc3cccc(F)c32)CC1)c1cccc(F)c1
SMILES(SDF)	c1cc(cc(c1)F)C(=O)NC2CCN(CC2)C(=O)Cn3c4c(cccc4F)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。

DLIP

PPI LIBRARY SEARCH

- Compound Search

ADVANCED SEARCH

- Physicochemical
- Druglikeness

CURATION SEARCH

- Compound Search
- Target Search

ABOUT

- About DB
- Analysis
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About DB

About PPI Library

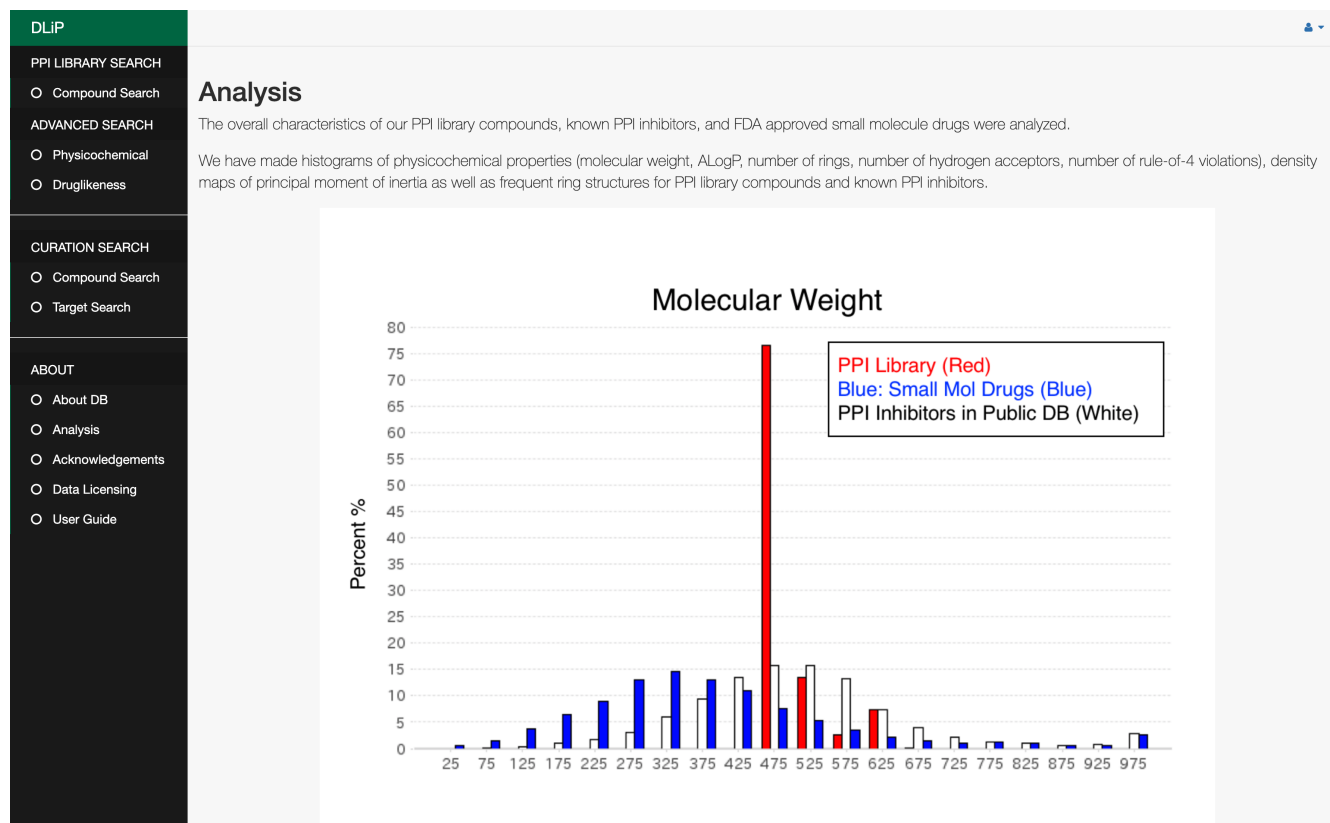
This database contains 15,000 compounds expected to PPI inhibitions and selected from a virtual compound library (K-Library developed by Kishida Chemical Co. Ltd., ~8M compounds). We conducted docking calculation against the virtual library on PDB structures of known PPI targets. Then, we selected and 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。

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

6.4. Data Licensing

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

DLiP	
PPI LIBRARY SEARCH	
<input type="radio"/> Compound Search	Academic users can freely use the DLiP database for non-profit aim. Non-academic users must contact us (dlipocontactus@gmail.com).
ADVANCED SEARCH	
<input type="radio"/> Physicochemical	Without any registration, everyone can login DLiP for evaluation by entering the following username and password.
<input type="radio"/> Druglikeness	- Sign in URL: /accounts/login/?username=anonymous&password=evaluation - Username: anonymous - Password: evaluation
CURATION SEARCH	
<input type="radio"/> Compound Search	
<input type="radio"/> Target Search	
ABOUT	
<input type="radio"/> About DB	
<input type="radio"/> Analysis	
<input type="radio"/> Acknowledgements	
<input type="radio"/> Data Licensing	
<input type="radio"/> User Guide	

6.5. User Guide

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

DLiP			
PPI LIBRARY SEARCH			
○ Compound Search			
ADVANCED SEARCH			
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○ Druglikeness			
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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 drug likeness (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。

