

統合データベース講習会：AJACS徳島 化合物データベース (Pubchem, ChEMBL) ～化合物情報とバイオアッセイ～

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 - 日時：2019年6月6日（木）
-

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2. 化合物データベース

- AJACS筑波 4 での化合物データベースについての説明へ
 - [Integbioデータベースカタログ](#)
 - https://github.com/AJACS-training/AJACS70/tree/master/03_yamada
-

3. 参考サイト

- 化合物の表記法やPubChemの使い方
 - ブラウザを用いた方法について
 - REST, SOAP, FTPによるデータ取得などについて
 - <https://github.com/yamadaissaku/ChemDocsJP>
 - <https://github.com/yamadaissaku/ChemInfo>
 - 統合TV
 - PubChemを利用して化学物質やアッセイの結果を調べる 2017
 - <https://tогotv.dbcls.jp/20171208.html>
-

4. PubChem

PubChemの説明

- [Web検索](#)
- PubChem公式
 - [pubchemdocs](#)

PubChem CompoundとSubstanceの違い



❖ Validate chemical contents

- Atoms defined/real
- Implicit hydrogen
- Functional group
- Atom valence



❖ Normalize representations

- Tautomer invariance
- Aromaticity detection
- Stereochemistry
- Explicit hydrogen



❖ Calculate

- 2-D depiction coordinates
- Molecular properties
- Chemical descriptors

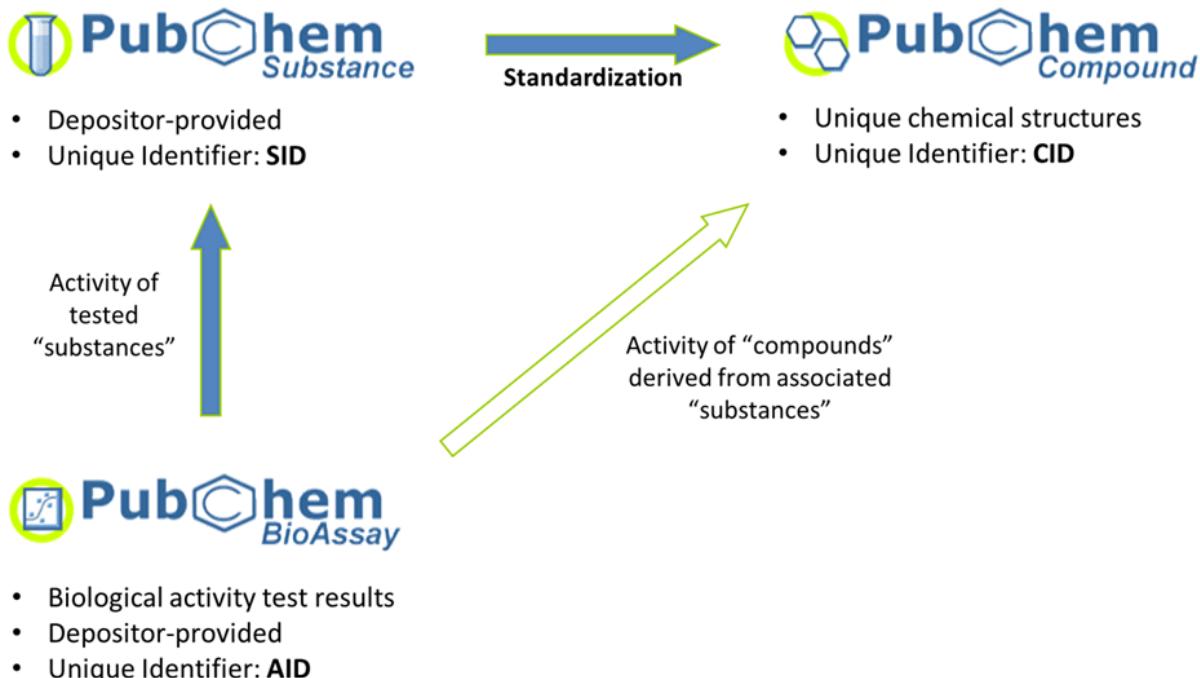


❖ Additional processing for mixtures

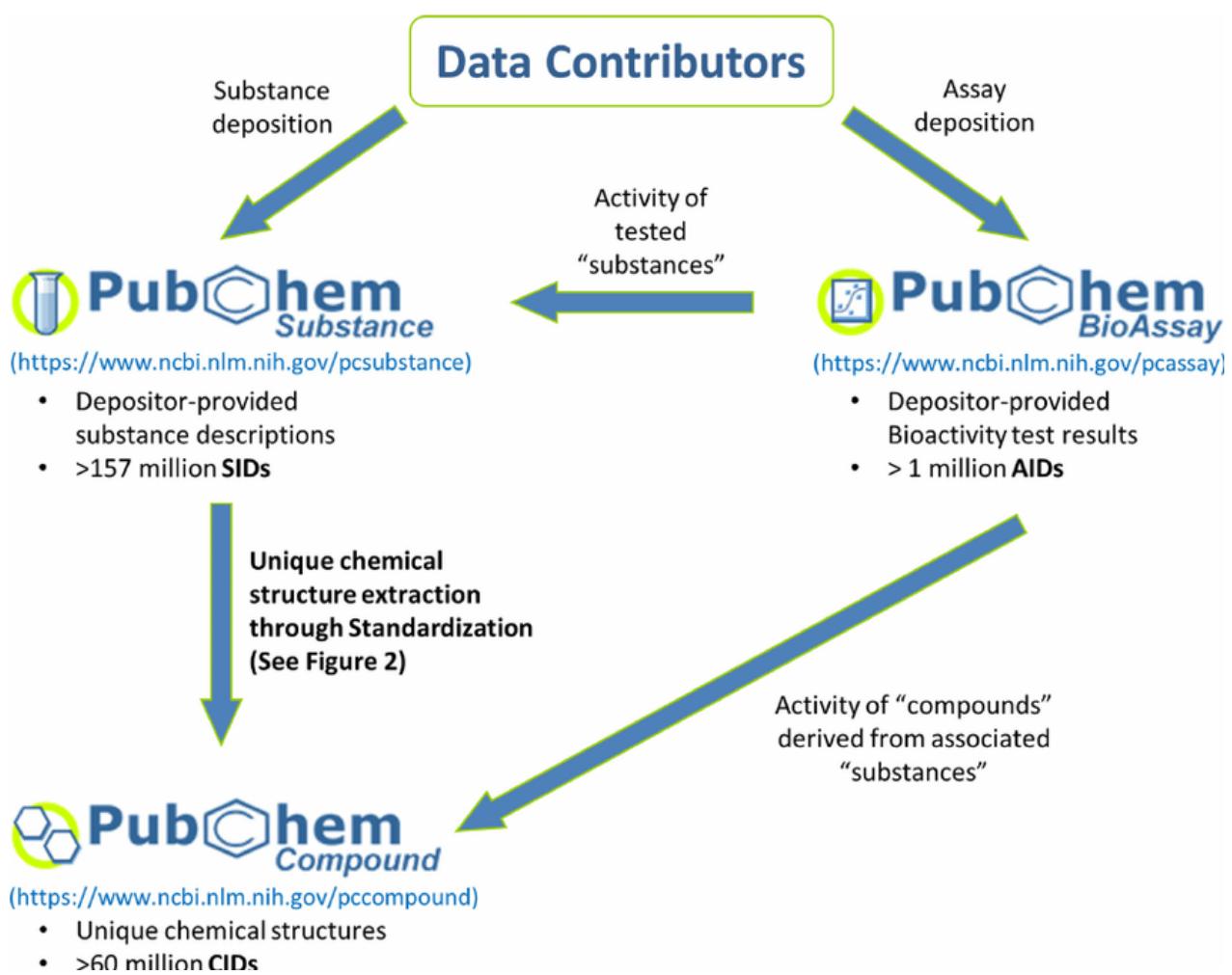
- Isolate covalent units
- Neutralize (by $\pm H^+$ or e^-)
- Reprocess
- Detect unique components



PubChem BioAssayとSubstance



PubChemへのデータ登録について



インターフェイスが今年3月に更新。

- <https://pubchemdocs.ncbi.nlm.nih.gov/about>

New Web Interface

Multiple updates to the PubChem web interface were released in March 2019.

PubChem About Blog Submit Contact | PubChem Periodic Table and Element pages [Read More >](#)

Explore Chemistry

Quickly find chemical information from authoritative sources

Search

Draw Structure

Upload ID List

Browse Data

Periodic Table

98M Compounds 245M Substances 266M Bioactivities 30M Literature 3M Patents [See More Statistics >](#)

671 Data Sources [Explore Data Sources >](#)

ウェブブラウザを用いた検索

キーワード検索から：遺伝子名：ACADM

1. 中鎖アシルCoAデヒドロゲナーゼ(MCAD)欠損症の病因遺伝子：ACADMについて調べてみましょう。
2. PubChemのサイト (<https://pubchem.ncbi.nlm.nih.gov/>) を開きます。
○ または、Googleなどの検索エンジンで"PubChem"と検索し、下記のリンクをクリック



<https://pubchem.ncbi.nlm.nih.gov/> このページを訳す

Search and explore chemical information in the world's largest freely accessible chemistry database.

RNAi BioAssays: 173 Tested Substances: 5,591,261

BioAssays: 1,067,566 Substances: 252,762,748

3. 下図のようにキーワード入力欄に"ACADM"を入力すると、Compound, Gene, Taxonomyに分類された候補キーワードが示されます。

Explore Chemistry

Quickly find chemical information from authoritative sources

ACADM

Compound	Gene	Taxonomy
ANACARDIC ACID	Acadm	Acaris
Meldrum's acid	Acam	Cutibacterium acnes
Tazobactam acid	ACAD8	Acalymma vittatum
BENZENEPENTACARBOXYLIC AC...	ACAD9	Acyrthosiphon pisum
Nalidixic acid sodium salt	Acadl	Stenostomum acutatum
Benzenehexacarboxylic acid	Acads	Colletotrichum acutatum
Acidum nicotinicum	Madm	Acanthamoeba quina
Acadyl	ACAN	Squalus acanthias
9,12-octadecadiynoic acid	ACAA1	Fusarium acuminatum
sulbactam acid	ACAA2	Achillea millefolium

98M Compounds 2451

[See More Statistics >](#)

676 Data Sources

[Explore Data Sources >](#)

4. 今回は、"Gene"の"Acadm"をクリックすると、下図のサイトに移動します。

5. ここでも、分類としてSubstances, Genes, BioAssays, Literature, Patentsが表示され、その下の()内に含まれるデータの数が表示されます。

SEARCH FOR

Acadm

Treating this query as a text search.

**Substances
(68)**

**Genes
(3)**

**BioAssays
(3)**

**Literature
(105)**

**Patents
(1)**

Searching chemical names and synonyms in the substance records submitted by PubChem's contributors. [Read More...](#)

68 results

[Filters](#)

SORT BY [Relevance](#)

[Download CSV](#)



[Search in Entrez](#)



ACTIONS ON RESULTS WITH ID TYPE:

- SID - Substances
 CID - Compounds

[Push to Entrez](#)

[Save for Later](#)

[Linked Data Sets](#)

[RNAi Of ACADM; Hs_ACADM_1; Hs_ACADM_5; GNF245219; GNF245220; ...](#)

Structure
not available

Substance SID: 85099111

Data Source: The Genomics Institute of the Novartis Research Foundation (GNF)

Data Source Category: Research and Development

Deposit Date: 2009-08-15 Last Modified Date: 2017-03-29

[RNAi Of ACADM; Hs_ACADM_2; Hs_ACADM_4; GNF245221; GNF245222; ...](#)

Structure
not available

Substance SID: 85106334

Data Source: The Genomics Institute of the Novartis Research Foundation (GNF)

Data Source Category: Research and Development

Deposit Date: 2009-08-15 Last Modified Date: 2017-03-29

6. ここで、"Gene"をクリックすると、taxonomy IDの異なる3個の遺伝子が含まれることがわかります。

- [9906: Homo sapiens \(human\)](#)
- [10090: Mus musculus \(house mouse\)](#)
- [10116: Rattus norvegicus \(Norway rat\)](#)

Substances (68) Genes (3) BioAssays (3) Literature (105) Patents (1)

Searching gene biological targets that have been tested in PubChem bioassays. [Read More...](#)

3 results SORT BY Relevance

ACADM - acyl-CoA dehydrogenase medium chain (human)
Gene ID: 34 Taxonomy ID: 9606
Gene Synonyms: ACADM; acyl-CoA dehydrogenase medium chain; ACAD1; MCAD; MCADH; ...
Linked BioAssays Count: 12

Acadm - acyl-Coenzyme A dehydrogenase, medium chain (house mouse)
Gene ID: 11364 Taxonomy ID: 10090
Gene Synonyms: Acadm; acyl-Coenzyme A dehydrogenase, medium chain; AU018656; MCAD; medium-chain specific acyl-CoA dehydrogenase, mitochondrial
Linked BioAssays Count: 3

Acadm - acyl-CoA dehydrogenase medium chain (Norway rat)
Gene ID: 24158 Taxonomy ID: 10116
Gene Synonyms: Acadm; acyl-CoA dehydrogenase medium chain; MCAD; medium-chain specific acyl-CoA dehydrogenase, mitochondrial; Acyl-Coenzyme A dehydrogenase, C-4 to C-12 straight-chain; ...
Linked BioAssays Count: 1

ACTIONS ON RESULTS WITH ID TYPE:
 GENEID - Genes
 AID - BioAssays
 TAXID - Taxonomy
 Push to Entrez
 Save for Later
 Linked Data Sets

7. ここで、各遺伝子毎にLinked BioAssays Countが表示されています。

Linked BioAssays Count: 12

8. Linked BioAssays Countのあとに数値、この場合は"12"をクリックすると、BioAssaysのサイトへ移動します。

PubChem ACADM - Acyl-CoA Dehydrogenase Medium Chain (Human) (Gene)

5 BioAssays

5.1 RNAi BioAssays

12 items View More Rows & Details

BioAssay AID	BioAssay Name	BioAssay Type
1904	siRNA Circadian Assay	Literature-derived
624099	An siRNA screen for human genes that are involved in human papilloma virus (HPV) E2 transcriptional repression of the E6 and E7 oncogenes	Other
651810	Genome-wide high-content siRNA screens for regulators of Parkin translocation in selective mitophagy (Dharmacon Library)	Screening
651811	Genome-wide high-content siRNA screens for regulators of Parkin translocation in selective mitophagy (Ambion Library)	Screening
743121	Druggable Genome siRNA Screen for Enhancers of Camptothecin in MDA-MB-231 Breast Cancer Cells	Screening

SORT BY Please Choose One

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- 4 Chemicals and Bioactivities
- 5 BioAssays
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- 9 Literature
- 10 Information Sources

from PubChem

9. Linked BioAssays Countのあとに数値、この場合は"12"をクリックすると、BioAssaysのサイトへ移動します。

- BioAssay AID, BioAssay Name, BioAssay Type の表示された表が表示されます。

5 BioAssays

5.1 RNAi BioAssays



をクリックすると、説明が表示されます。この機能はPubChemの色々なサイトにありますので、"これ何?"と思ったら、クリックしてみてください。

5 BioAssays



Biological experiments deposited in PubChem BioAssay that were conducted against this target

5.1 RNAi BioAssays



Functional genomic bioassays that tested RNAi reagents

10. 右上のDownloadをクリックとCSV形式で取得することができます。ダウンロードしたCSV形式のファイルを開くと以下のようにになります。

aid	aidtype	aidname	aiddesc	aidsrcid	aidsrcname	aidmdate	cids	sids	geneids	aidcategory	protacns	depcatg	pmids	rmai	dois
1904	100	siRNA Circad Description:		37	The Genomic	20100701	NULL	85098869,851,2,9,10,12,1	RNAi	NULL	resdev	19765810	1	10.1016/j.cell.2	
624099	0	An siRNA scr An essential		46	ICCB-Longwi	20161014	NULL	56478464,561,2,9,10,12,1	RNAi	NULL	resdev	#####	1	10.1073/pnas.C	
651810	1	Genome-wid High-content		2	NCGC	20131202	NULL	56478465,561,2,9,10,12,1	RNAi	NULL	government,r	24270810	1	10.1038/nature	
651811	1	Genome-wid High-content		2	NCGC	20131210	NULL	160713784,1,1,2,9,10,12,1	RNAi	NULL	government,r	24270810	1	10.1038/nature	
743121	1	Druggable G/Camptothecin		2	NCGC	20140721	NULL	164351727,1,1,2,12,13,18,	RNAi	NULL	government,r	NULL	1	NULL	
743454	1	RNAi screen Assay descrip		68	Victorian Cer	20160302	NULL	56478465,561,2,9,10,12,1	RNAi	NULL	resdev	25977774	1	10.1038/sdata.	
1117281	1	A whole gen Immunotoxin		2	NCGC	20150316	NULL	160713784,1,1,2,9,10,12,1	Toxicity, RNA	NULL	government,r	25713356	1	10.1073/pnas.1	
1117357	1	InfectX: Path Pathogen inf		71	InfectX Cons	20160304	NULL	249376050,2,1,2,9,10,12,1	RNAi	NULL	resdev	26445817	1	10.1186/s1305	
1159506	0	Identification Ewing sarcom		2	NCGC	20160129	NULL	160713784,1,1,2,9,10,12,1	Cell-based,R	NULL	government,r	NULL	1	NULL	
1159578	1	A screen to ic Genome wide		68	Victorian Cer	20161215	NULL	255348109,2,1,2,9,10,12,1	RNAi	NULL	resdev	NULL	1	NULL	
1159584	1	A screen to ic Genome wide		68	Victorian Cer	20160303	NULL	56478465,561,2,9,10,12,1	RNAi	NULL	resdev	25777964	1	10.1158/1535-	
1224830	3	Genome-wid The mammal		79	Iain Fraser	20170223	NULL	315447116,3,1,2,9,10,12,1	RNAi	NULL	resdev	NULL	1	NULL	

11. テーブルの”BioAssay AID”をクリックすると、以下のようなアッセイの詳細を見ることができます。

NIH U.S. National Library of Medicine
National Center for Biotechnology Information



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Search PubChem

BIOASSAY RECORD

Genome-wide high-content siRNA screens for regulators of Parkin translocation in selective mitophagy (Dharmacon Library)

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[Cite](#)

[Download](#)

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Title and Summary

1 Description

2 Data Table

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5 Information Sources

PubChem AID:	651810
Primary Citation:	High-content genome-wide RNAi screens identify regulators of parkin upstream of mitophagy. [PMID: 24270810]
Source:	NCGC
External ID:	Parkin-RNAi-Dharmacon
BioAssay Type:	Primary Screening
Substance Type:	Nucleotide
Tested Substances:	All (18,119) Active (826) Inactive (17,293) Data Table
Version:	2.4
Status:	Live
Dates:	Modify: 2013-12-02 Hold-Until: 2013-11-24 Deposit: 2012-11-27
This bioassay record (AID 651810) reports results from the above primary citation.	
from PubChem	

12. 詳細ページには上図のようなことが記載されています。

- "Tested Substances:"を見ていただくと、"Active"と"Inactive"の件数がわかります。

■ "Data table"をクリックすると下記のTableが表示されます。これは、ページをスクロールすることや、ページ右端の"CONTENTS"の"2 Data Table"をクリックすることでも同様に移動できます。

2 Data Table



18,119 tested substances

[Download](#)

Tested Substance	Activity	Score	Vendor Supplied Gene Symbol	Raw Sample Value	Median Negative Control on Plate	Median Positive Control on Plate	PPT Sample as Percentage of Negative Control	PPT MAD Z-Score	P	
									N	M
SID										
152153881	Active	100	STK11	19.3548	38.6229	93.3125	50.1124	-1.39251	-	
152155875	Active	100	SPTBN1	65.3114	21.7866	90.03	299.777	3.41306	2	
152148934	Active	100	PAFAH1B1	34.2547	9.53179	92.239	359.373	4.56017	2	
134310598	Active	100	EHD3	17.1353	34.3386	94.6928	49.901	-1.39658	-	
134316848	Active	100	LMX1B	16.3297	36.484	94.2952	44.7585	-1.49556	-	

1 2 3 ... 3,624 Next >

▶ from PubChem

13. 右上の”?”をクリックするとここでも説明が表示されます。

2 Data Table

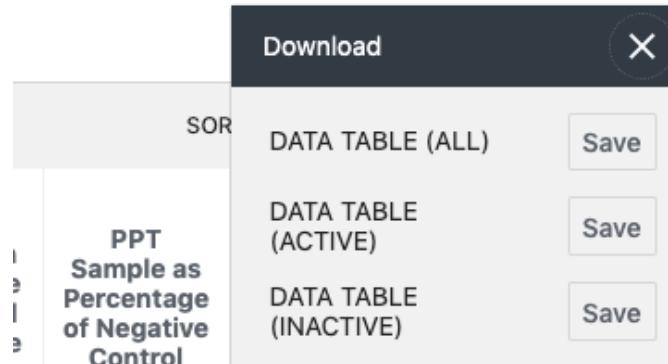


Biological test results provided by depositor. The column highlighted in bold (if any) indicates the active concentration (AC). Subset data for probe substances, active substances, inactive substances, substances with AC <= 1uM, or substances with AC <= 1nM is provided under certain tab (if any). The complete data or subset data can be downloaded via the "Download". Click the chemical structure or outcome column linking to the bioactivity summary page for each bioassay-substance pair. Click the "Refine/Analyze" for available tools to analyze the bioactivity data. "SAR Analysis" provides structure-activity analysis via a heatmap display for the active compounds

14. Data Tableには様々な情報が登録されています。右上の”SORT BY”的プルダウンにより、Activity, Score, SID, CID

Tested Substance	Activity	Score	Vendor Supplied Gene Symbol	Raw Sample Value	Median Negative Control on Plate	Choose Sort Options	
						Activity	Score
SID						SID	CID

15. 右上のDownloadをクリックとCSV形式で取得することができます。また、Data Tableのダウンロードでは、下図のようにALL, ACTIVE, INACTIVEをそれぞれ取得できます。



16. 取得したCSV形式のファイルを開くと以下のようにになります。

RESULT_TYPE	RESULT_UNIT	PUBCHEM_R	PUBCHEM_S	PUBCHEM_C	PUBCHEM_A	PUBCHEM_P	PUBCHEM_V	Vendor Supp	Raw Sample	Median Neg	Median Pos	PPT Sample	PPT MAD Z	PPT Log	MAI	Cell Count	S	Median Neg	Median Pos	Sample Cell	(Sample
						STRING	FLOAT	FLOAT	FLOAT	FLOAT	FLOAT	FLOAT	INTEGER	FLOAT	FLOAT	FLOAT	FLOAT	FLOAT	FLOAT	FLOAT	
1	56478550	Active	100	ROR2	16.3034	38.6229	93.3125	42.2118	-1.54458	-2.43828	1024	1275	1010.5	-0.320121	44						
2	56478596	Active	100	CDK2	16.4716	38.8317	94.1628	42.4179	-1.54062	-2.42712	1062	1361	968	-0.520005	35						
3	56478616	Active	100	E2F1	34.689	10.1407	91.6574	342.078	4.22726	2.35175	753	1329.5	1048.5	-2.39315	20						
4	56478630	Active	100	ORC6L	14.1713	33.2009	94.8342	42.6835	-1.5355	-2.41283	1098	1114	949	1.27782	41						
5	56478651	Active	100	TP73L	64.7306	18.4552	90.6847	350.745	4.39409	2.40903	1286	1456.5	1165.5	0.378608	33						
6	56478759	Active	100	CAMK2D	17.5972	37.237	92.7941	47.2573	-1.44747	-2.1798	1333	1234	1031	2.10604	46						
7	56478765	Active	100	PANK1	15.3673	37.237	92.7941	41.269	-1.56273	-2.48999	1214	1234	1031	1.26167	39						
8	56478975	Active	100	TRPM6	15.5657	37.237	92.7941	41.8017	-1.55248	-2.46063	1179	1234	1031	1.01333	38						
9	56478976	Active	100	ULK1	19.3053	38.8317	94.1628	49.7154	-1.40015	-2.06371	1118	1361	968	-0.159735	33						
10	56479093	Active	100	DGKI	18.7215	38.6229	93.3125	48.4725	-1.42408	-2.12167	1137	1275	1010.5	0.455889	38						
11	56479094	Active	100	DGK2	18.4141	36.0002	94.9202	51.15	-1.37254	-1.99858	996	1060.5	948.5	0.871047	49						
12	56479184	Active	100	MGC5601	84.7973	21.8358	91.9146	388.341	5.11774	2.64214	1030	1416.5	1136.5	-0.985504	29						
13	56479268	Active	100	CDK5RAP1	65.1254	21.8358	91.9146	298.251	3.38368	2.03787	1009	1416.5	1136.5	-1.11531	30						
14	56479273	Active	100	GK2	19.1781	38.8317	94.1628	49.3878	-1.40646	-2.07885	1018	1361	968	-0.803075	27						
15	134309828	Active	100	MAD2L1	64.2424	21.7866	90.03	294.871	3.31862	2.01178	1019	1430	1177.5	-1.11296	28						
16	134309847	Active	100	KIF14	70.7921	20.7811	91.2401	340.656	4.19989	2.34221	718	1423.5	1155.5	-0.39591	45						
17	134309878	Active	100	NR4A2	66.3979	18.4552	90.6847	359.779	4.56798	2.46725	1055	1456.5	1165.5	-1.01007	47						
18	134309929	Active	100	HDAC6	62.8392	19.5679	90.8493	321.134	3.82414	2.20711	1328	1429.5	1158	0.781882	42						

17. Data Tableからのリンクは、SID, Activity, Entrez GeneIDから、それぞれのページに移動することができます。

18. Data Tableの各列のSIDのSID（例えば：152153881）をクリックすると下図のようなページが表示されます。

Tested Substance

SID

152153881
152155875
152148934
134310598

NIH U.S. National Library of Medicine

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SUBSTANCE RECORD

M-005035-02

PubChem SID: 152153881

Source: Dhamacon, a Horizon Discovery Group company

External ID: M-005035-02

Source Category: siRNA Reagent Vendors

Version: 2 Revision History

Status: Live

Dates: Modify: Available: Deposit:
2015-05-15 2012-11-03 2012-11-03

Please note that the substance record is presented as provided to PubChem by the source (depositor).

from PubChem

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Cite Download

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- Title and Summary
- 1 Identity
- 2 Depositor Comments
- 3 Biological Test Results
- 4 Entrez Crosslinks
- 5 Information Sources

19. このページでは、Depositor CommentsやSIDに関するBiological Test Resultsを得ることができます。

2 Depositor Comments



siGENOME SMARTpool siRNA reagent, GE Healthcare Dharmacon catalog number M-005035-02, targeting serine/threonine kinase 11 (STK11). Designed to target all coding transcript variants of its target gene known at time of design. Developed for RNA interference (RNAi); reagent is available at [dharmacon.gelifesciences.com/rnai-and-custom-rna-synthesis/](http://dharmacon.gelifesciences.com/rnai-and-custom-rna-synthesis).

▶ from PubChem

3 Biological Test Results



3.1 BioAssay Results



32 items

View More Rows & Details

Download

BIOASSAY RECORD > BIOACTIVITY DYAD					
Activity	Activity Value, μM	Activity Type	Target Name	BioAssay Name	BioAssay AID
Active			STK11 - serine/threonine kinase 11 (human)	Genome-wide high-content siRNA screens for regulators of Parkin translocation in selective mitophagy (Dharmacon Library)	651810
Inactive			STK11 - serine/threonine kinase 11 (human)	AT1R-EGFR transactivation kinome screen - primary	720703
Active			STK11 - serine/threonine kinase 11 (human)	RNAi screen for vorinostat resistance genes - Primary Screen	743454
Inactive			STK11 - serine/threonine kinase 11 (human)	Human kinome siRNA screen in A549-BTR and MDA-231-1833-BTR cells	1117269
Inactive			STK11 - serine/threonine kinase 11 (human)	A screen to identify synthetic lethal interactions with E-cadherin in an MCF10A isogenic cell line	1159584

1 2 3 ... 7 Next >

20. Data Tableの各列のActivityのActive or Inactiveをクリックすると下図のようなページが表示されます。

Activity
Active
Active
Active

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BIOASSAY RECORD > BIOACTIVITY DYAD

Bioactivity for AID 651810 - SID 152155875

PubChem Bioactivity: AID 651810 - SID 152155875

This page summarizes the biological test results for the substance siGENOME SMARTpool siRNA reagent for SPTBN1 (SID 152155875) tested in the bioassay Genome-wide high-content siRNA screens for regulators of Parkin translocation in selective mitophagy (Dharmacon Library) (AID 651810). The same substance was also tested in other bioassays.

▶ from PubChem

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- Title and Summary**
- 1 PubChem SID
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- 5 Information Sources



3 Test Results

23 items [View More Rows](#)
 [Download](#)

TID	Name	Test Results	Unit	AC	Description	Type
1	Vendor Supplied Gene Symbol	SPTBN1				STRING
2	Raw Sample Value	65.3114	none			FLOAT
3	Median Negative Control on Plate	21.7866	none			FLOAT
4	Median Positive Control on Plate	90.03	none			FLOAT
5	PPT Sample as Percentage of Negative Control	299.777	none			FLOAT

1 2 3 ... 5 [Next >](#)

4 Related Bioactivities



Other bioactivity data found in PubChem BioAssay

4.1 Other BioAssays



Other bioassays that tested the same substance

2 items [Download](#)

Activity	Activity Type	Activity Value, μM	BioAssay AID	BioAssay Name
Inactive			743454	RNAi screen for vorinostat resistance genes - Primary Screen
Inactive			1159584	A screen to identify synthetic lethal interactions with E-cadherin in an MCF10A isogenic cell line

21. Data Tableの各列のEntrez GenelDをクリックすると下図のようなページが表示されます。このページでは、遺伝子に関する各種情報をることができます。

Entrez GenelD

[6794](#)[6711](#)[5048](#)[30845](#)



GENE SUMMARY

PAFAH1B1 - platelet activating factor acetylhydrolase 1b regulatory subunit 1 (human)

NCBI Gene:	5048
Symbol:	PAFAH1B1
Taxonomy:	Homo sapiens (human)
	LIS1 LIS2 MDCR MDS NudF
Synonyms:	More...
Dates:	Modify: 2019-03-15 Create: 2016-09-14

This locus was identified as encoding a gene that when mutated or lost caused the lissencephaly associated with Miller-Dieker lissencephaly syndrome. This gene encodes the non-catalytic alpha subunit of the intracellular 1b isoform of platelet-activating factor acetylhydrolase, a heterotrimeric enzyme that specifically catalyzes the removal of the acetyl group at the SN-2 position of platelet-activating factor (identified as 1-O-alkyl-2-acetyl-sn-glyceryl-3-phosphorylcholine). Two other isoforms of intracellular platelet-activating factor acetylhydrolase exist: one composed of multiple subunits, the

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Title and Summary

1 Names and Identifiers

2 Related Genes

3 Proteins

4 BioAssays

5 Diseases and Phenotypes

6 Classification

7 Interactions and Pathways

8 Literature

9 Information Sources

URLへキーワード（遺伝子名、生物種など）を用いた検索

- 以下のようなURLを用いることで、キーワードに該当するエントリーを表示させることができます。

- <https://pubchem.ncbi.nlm.nih.gov/gene/ACADM/human>



GENE SUMMARY

ACADM - acyl-CoA dehydrogenase medium chain (human)

NCBI Gene:	34
Symbol:	ACADM
Taxonomy:	Homo sapiens (human)
	ACAD1 MCAD MCADH
Synonyms:	medium-chain specific acyl-CoA dehydrogenase, mitochondrial acyl-CoA dehydrogenase, C-4 to C-12 straight chain
	More...
Dates:	Modify: 2019-03-15 Create: 2016-09-14

This gene encodes the medium-chain specific (C4 to C12 straight chain) acyl-Coenzyme A dehydrogenase. The homotetramer enzyme catalyzes the initial step of the mitochondrial fatty acid beta-oxidation pathway. Defects in this gene

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9 Literature

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PROTEIN SUMMARY

Epidermal growth factor receptor

NCBI Protein: P00533

Encoding Gene: EGFR

Taxonomy: Homo sapiens (human)

Dates: Modify: 2019-03-20 Create: 2017-04-15

Receptor tyrosine kinase binding ligands of the EGF family and activating several signaling cascades to convert extracellular cues into appropriate cellular responses (PMID: 2790960, PMID: 10805725, PMID: 27153536). Known ligands include EGF, TGFA/TGF-alpha, AREG, epigen/EPGN, BTC/betacellulin, epiregulin/EREG and HBEGF/heparin-binding EGF (PMID: 2790960, PMID: 7679104, PMID: 8144591, PMID: 9419975, PMID: 15611079, PMID: 12297049, PMID: 27153536, PMID: 20837704). Ligand binding triggers receptor homo- and/or heterodimerization and autophosphorylation on key cytoplasmic residues. The phosphorylated receptor recruits adapter proteins like GRB2 which in turn activates complex downstream signaling pathways.

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[Cite](#)
[Download](#)

CONTENTS

Title and Summary

1 Names and Identifiers

2 Related Proteins

3 Chemicals and Bioactivities

4 BioAssays

5 Sequence

6 3D Structures

7 Domains

8 Literature

9 Information Sources

PubChem Classification Browserを使ったデータ取得

- 下記の検索ボックス下にあるアイコンの右から二番目の"Browse Data"をクリックします。
 - または、下記のURLへ移動します。

<https://pubchem.ncbi.nlm.nih.gov/classification/#hid=1>



Explore Chemistry

Quickly find chemical information from authoritative sources

Search

Try aspirin EGFR C9H8O4 57-27-2 C1=CC=C(C=C1)C=O InChI=1S/C3H6O/c1-3(2)4/h1-2H3



Draw Structure



Upload ID List



Browse Data



Periodic Table

- 下図のようなClassification Browserが表示されます。

NCBI

PubChem Classification Browser

Help

Browse PubChem data using a classification of interest, or search for PubChem records annotated with the desired classification/term (e.g., MeSH: phenylpropionates, or Gene Ontology: DNA repair). More...

Select classification Search selected classification by

MeSH Keyword Enter desired search term **Search**

Classification description (from MeSH)
MeSH (Medical Subject Headings) is the NLM controlled vocabulary thesaurus used for indexing articles for PubMed. More...

Data type counts to display Display zero count nodes?

None Compound Substance PubMed Yes No

Browse MeSH Tree

- ▼ MeSH Tree ? 126,919
 - ▶ Analytical, Diagnostic and Therapeutic Techniques and Equipment Category
 - ▶ Anatomy Category
 - ▶ Anthropology, Education, Sociology and Social Phenomena Category
 - ▶ Chemicals and Drugs Category ? 126,919
 - ▶ Disciplines and Occupations Category

3. Select classificationで、"ChEMBL"を選択してください。

NCBI

PubChem Classification Browser

Help

Browse PubChem data using a classification of interest, or search for PubChem records annotated with the desired classification/term (e.g., MeSH: phenylpropionates, or Gene Ontology: DNA repair). More...

Select classification Search selected classification by

ChEMBL Keyword Enter desired search term **Search**

Classification description (from ChEMBL)
The ChEMBL Protein Target Tree is a structured classification of the protein target entities contained with the ChEMBL resource.
Author: ChEMBL curation team
ChEMBL Release version 24
For any queries contact chembl-help@ebi.ac.uk
Created on 05/01/2019 09:02:54 More...

Data type counts to display Display zero count nodes?

None Compound Substance Assay PubMed Gene Protein Taxonomy Yes No

Browse ChEMBL Tree

- ▼ Target Tree ? 750,864
 - ▶ Auxiliary transport protein 838
 - ▶ Enzyme ? 393,970
 - ▶ Epigenetic regulator ? 16,806

1. Data type counts to display の下に、None, Compound, Substance, Assay, PubMed, Gene, Protein, Taxonomy が表示されました。

None Compound Substance Assay PubMed Gene Protein Taxonomy

2. AssayやGeneを選択すると、以下のように項目に含まれる数値が変わります。

Data type counts to display

None	Compound	Substance	Assay	PubMed	Gene	Protein	Taxonomy
------	----------	-----------	-------	--------	------	---------	----------

Browse ChEMBL Tree

- ▼ Target Tree ? ↗ 5,519
- ▶ Auxiliary transport protein 29
 - ▶ Enzyme ? 2,960
 - ▶ Epigenetic regulator ? 120
 - ▶ Ion channel ? 369

3. 左の青三角をクリックすると下の階層が表示されます。

- ▼ Target Tree ? ↗ 5,519
- ▼ Auxiliary transport protein 29
 - Ankyrin family
 - Basigin family
 - Calcium channel auxiliary subunit alpha2delta family 6
 - Calcium channel auxiliary subunit beta family 4
 - Calcium channel auxiliary subunit gamma family 8

4. 右の青い数字をクリックすると、リストが表示されます。

Tabular ▾ 20 per page ▾ Sort by Relevance ▾ Send to: ▾ Hide sidebar >>

Links from pchierarchy

Items: 1 to 20 of 29

<< First < Prev Page 1 of 2 Next > Last >>

Filter: Manage Filters

Results by taxon

Top Organisms [Tree]

- Homo sapiens (26)
- Rattus norvegicus (1)
- Mus musculus (1)
- Bos taurus (1)

Find related data

Database: Select

Find items

Recent activity

Name/Gene ID	Description	Location	Aliases	MIM
<input checked="" type="checkbox"/> KCNMB1 ID: 407176	potassium calcium-activated channel subfamily M regulatory beta subunit 1 [Bos taurus (cattle)]	Chromosome 20, NC_037347.1 (2256775..2269577, complement)		
<input checked="" type="checkbox"/> CACNA2D4 ID: 93589	calcium voltage-gated channel auxiliary subunit alpha2delta 4 [Homo sapiens (human)]	Chromosome 12, NC_000012.12 (1791957..1922606, complement)	RCD4	608171
<input checked="" type="checkbox"/> CACNG6 ID: 50285	calcium voltage-gated channel auxiliary subunit gamma 6 [Homo	Chromosome 19, NC_000019.10		606898

5. 左上のプルダウンで、Format, 表示件数、ソートを変更できます。

Tabular ▾ 20 per page ▾

Format	Items per page	Sort by
<input checked="" type="radio"/> Summary <input type="radio"/> Summary (text) <input checked="" type="radio"/> Tabular <input type="radio"/> Tabular (text) <input type="radio"/> ASN.1 <input type="radio"/> XML <input type="radio"/> UI List	Tabular ▾ 20 per page ▾ <ul style="list-style-type: none"> 5 10 20 <input checked="" type="radio"/> 50 100 200 	Page ▾ Sort by Relevance ▾ <ul style="list-style-type: none"> Relevance <input checked="" type="radio"/> Gene Weight Name Chromosome

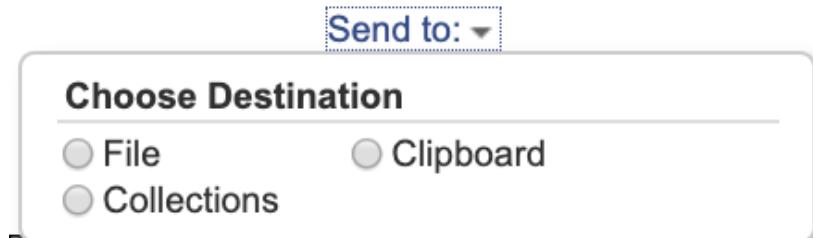
6. 左の Results by taxonから、生物種を選択して絞り込みができます。

Results by taxon

Top Organisms [Tree]

- Homo sapiens (26)
- Rattus norvegicus (1)
- Mus musculus (1)
- Bos taurus (1)

7. 検索（選択）されたリストは右上の"Send to:"のプルダウンから、形式を選択してデータ得ることができます。



5. ChEMBL

ChEMBLの説明

- ChEMBLとは
 - ChEMBLはEBIのChEMBLチームにより維持管理されている化合物の活性などを収録したデータベース
 - 以下のリンクも参考になります。
 - https://github.com/Mishima-syk/py4chemoinformatics/blob/master/ch04_database.asciidoc
- ChEMBL Interface Questions
 - <https://chembl.gitbook.io/chembl-interface-documentation/frequently-asked-questions/chembl-interface-questions#can-i-edit-the-query-being-used>
- chembl-interface-documentation
 - <https://chembl.gitbook.io/chembl-interface-documentation/>

ウェブブラウザを利用して

1. ChEMBLのサイト（<https://www.ebi.ac.uk/chembl/>）を開く
 - または、Googleなどの検索エンジンで"ChEMBL"と検索し、下記のリンクをクリック

ChEMBL Database - EMBL-EBI

<https://www.ebi.ac.uk/chembl/> ▼ このページを訳す

The ChEMBL database in 2017. Gaulton A, Hersey A, Nowotka M, Bento AP, Chambers J, Mendez D, Mutowo P, Atkinson F, Bellis LJ, Cibrián-Uhalte E, Davies M, Dedman N, Karlsson A, Magariños MP, Overington JP, Papadatos G, Smit I, ...

[ChEMBL logo](#) · [Database Schema](#) · [Dopamine](#) · [WS Diagram](#)

2. 概要

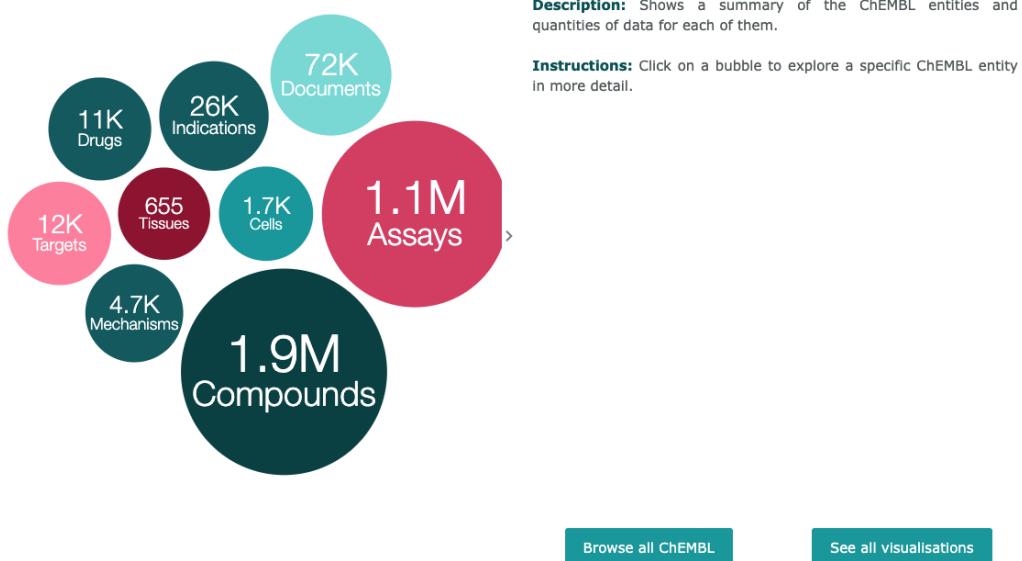
含まれるデータの俯瞰

- 左図の"＜", "＞"をクリックすると、表示される項目が以下のようにかわります。

The screenshot shows the ChEMBL homepage with a teal header. The header includes links for EMBL-EBI, Services, Research, Training, About us, and a search bar with examples like Dopamine, HepG2, NAFRONYL, CC(=O)..., Draw a Structure, and Enter a Sequence. Below the header are links for UniChem, ChEMBL-NTD, SureChEMBL, Downloads, Web Services, Old Interface, and More.

ChEMBL is a manually curated database of bioactive molecules with drug-like properties. It brings together chemical, bioactivity and genomic data to aid the translation of genomic information into effective new drugs.

Explore ChEMBL



Current Release: ChEMBL 25
Provided under a Creative Commons Attribution-ShareAlike 3.0 Unported license
Last Update on 2018-12-10 | [Release notes](#)



12,482
Targets



1,879,206
Distinct compounds



15,504,603
Activities

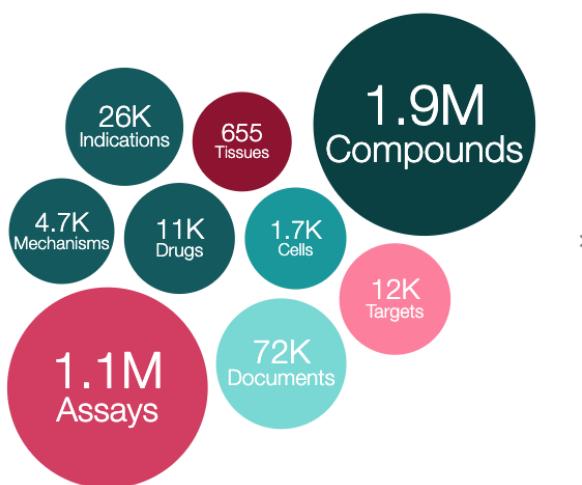


72,271
Publications



54
Deposited Datasets

Explore ChEMBL



Description: Shows a summary of the ChEMBL entities and quantities of data for each of them.

Instructions: Click on a bubble to explore a specific ChEMBL entity in more detail.

[Browse all ChEMBL](#)

[See all visualisations](#)

階層

- 表示された項目をクリックすることで下の階層を見ることができます。



Protein Targets in ChEMBL

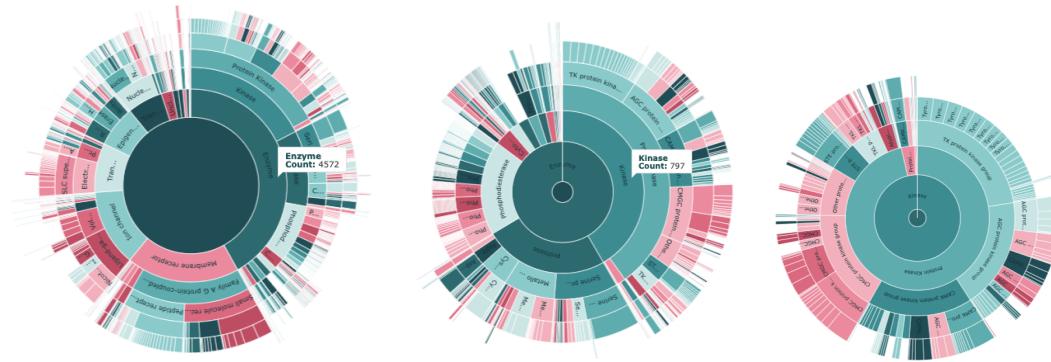
Description: Representation of the ChEMBL protein target classification hierarchy.

Instructions: Click on a section to expand it and then click on the browse button to start exploring the target family in more detail.

[Browse all Targets](#)

[See all visualisations](#)

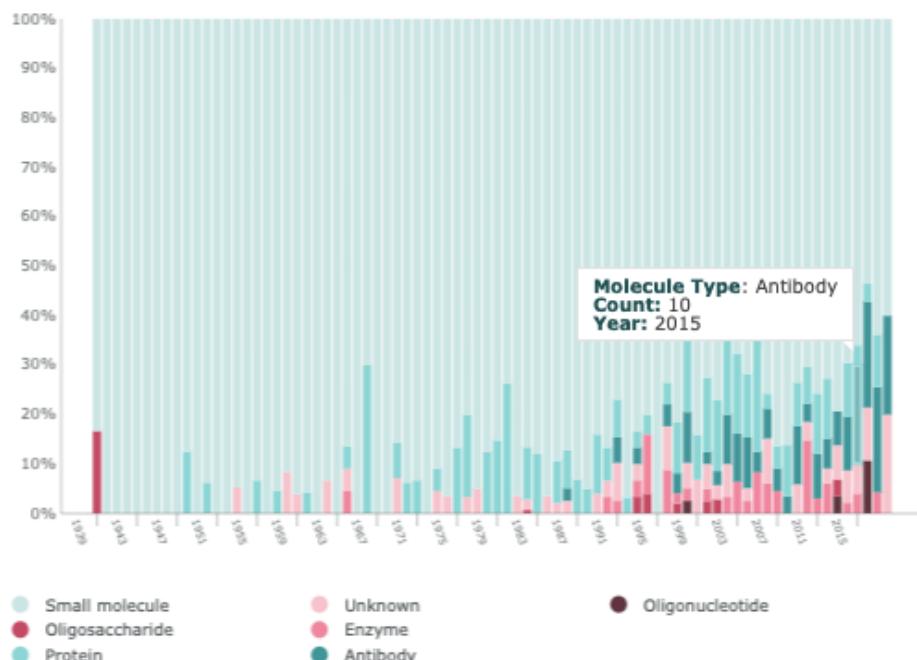
- "Enzyme"をクリックすると下図（中央）のように下の階層を見ることができます。
- さらに"Kinase"をクリックすると下図（右）のように下の階層を見ることができます。



年代毎の分子の種類の分布

- マウスオーバーするとデータが表示されます。

Drugs By Molecule Type and First Approval (1973)



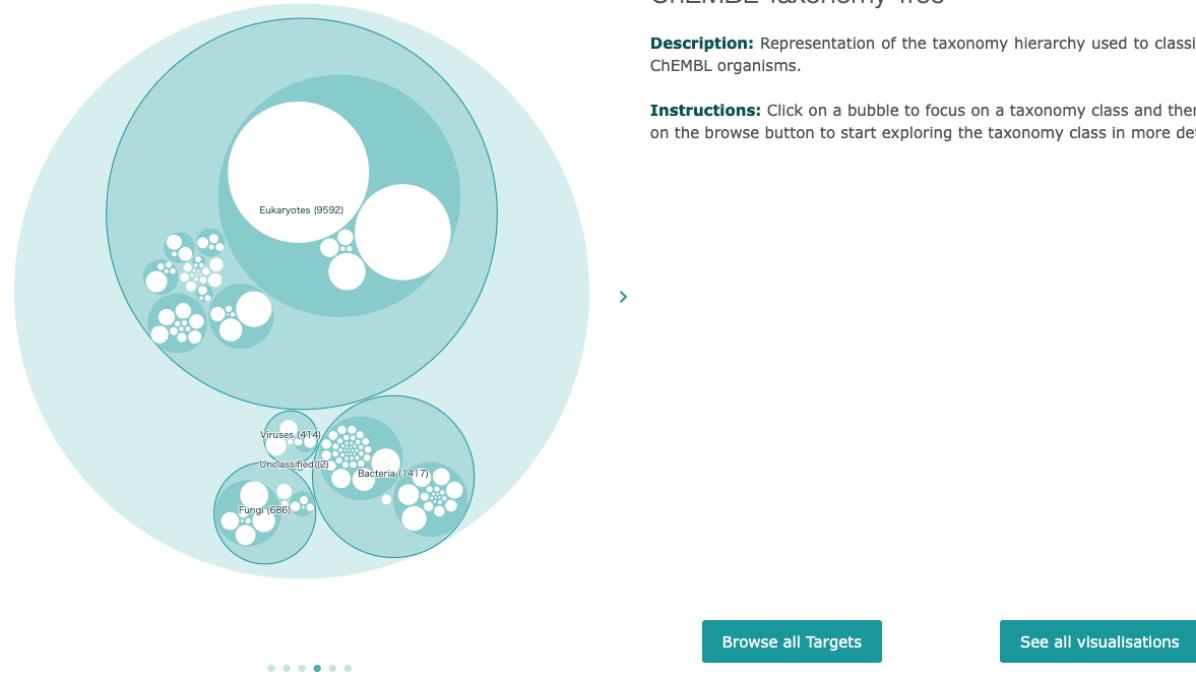
Taxonomyによる分類

- クリックして中を見ていくことができます。

ChEMBL Taxonomy Tree

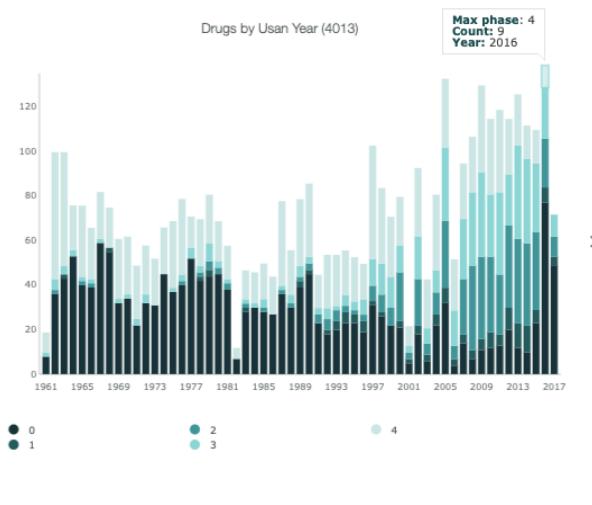
Description: Representation of the taxonomy hierarchy used to classify the ChEMBL organisms.

Instructions: Click on a bubble to focus on a taxonomy class and then click on the browse button to start exploring the taxonomy class in more detail.



開発フェーズとUSAN登録

- マウスオーバーして、クリックするとその情報が表示されます。



Development Phase and USAN Registration

Description: Bar chart showing the current maximum development phase for compounds and the year they were registered with a USAN (United States Adopted Name). Note: only shows compounds with a known USAN registration year.

Instructions: Click on a bar to explore the drugs' details.

ChEMBL

Search in ChEMBL

Edit Querystring [?](#)
Show Full Query [?](#)

Table Cards Graph Heatmap

9 Drugs
0 Selected - Select All
Browse Activities [?](#)

CSV TSV SDF

Filters Showing 1-9 out of 9 records

Type
Max Phase
#RO5 Violations
Molecular Weight
AlogP
Is Drug
ATC Class. Level 1
ATC Class. Level 2
Targets
Bioactivities

Records per page:
24

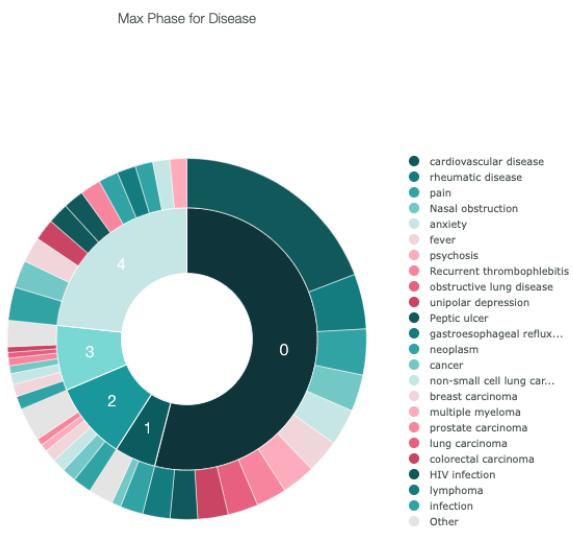
CHEMBL3707372
Synonyms:
+ Voxilaprevir (FDA, INN, USAN)
Research Codes: GS-9857
Max Phase: 4

CHEMBL3989866
Synonyms:
+ Bictegravir (FDA, INN, USAN)
Research Codes: GS-9883, GS-9883-01
Max Phase: 4

CHEMBL3707348
Synonyms:
+ Acalabrutinib (FDA, INN, USAN)
Research Codes: ACP-196
Max Phase: 4

CHEMBL408403
Synonyms:
+ Angiotensin II (INN, JAN, USAN)
Research Codes:
Max Phase: 4

病気のフェーズ



ChEMBL Indications for Drugs

Description: Distribution of drugs and clinical candidate development phases for the most frequent drug indications. Note: less frequently occurring indications are not shown.

Instructions: Click on a sector of the piechart to explore the compounds for that indication and development phase.

Browse all Drugs

See all visualisations

- 色のついたところをクリックすると下図のような関連する化合物リストが表示されます。

Browse Compounds

[Edit Querystring](#) [Show Full Query](#)

Table Cards Graph Heatmap

2,713 Compounds
0 Selected - Select All
[Browse Activities](#)

[CSV](#) [TSV](#) [SDF](#)

Showing 1-24 out of 2,713 records

Records per page: 24 Select All

Type	Count
Antibody	80
Cell	1
Enzyme	43
Oligonucleotide	7
Oligosaccharide	15
Protein	190
Small molecule	2258
Unknown	119

Max Phase	Count
4	2713

#RO5 Violations	Count
0	1519
1	270
2	147
3	38
4	3

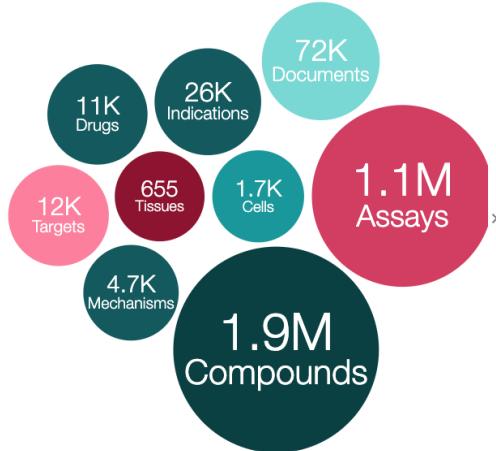
CHEMBL1201620
Name: SOMATREM

CHEMBL2108117
Name: SITOSTEROLS

CHEMBL2108809
Name: SULESOMAB

CHEMBL2109079
Name: HYETELLOSE

化合物



- Compoundsをクリックすると下図のような化合物リストが表示されます。

Browse Compounds

[Edit Querystring](#)
[Show Full Query](#)

Table Cards Graph Heatmap

1,879,206 Compounds
0 Selected - Select All
Browse Activities

CSV TSV SDF

Showing 1-24 out of 1,879,206 records

Records per page: 24

Select All

Filters	
▲ Type	
+ Antibody	736
- Cell	29
- Enzyme	99
- Oligonucleotide	111
- Oligosaccharide	63
- Protein	22537
Small molecule	1849655
- Unclassified	4
- Unknown	5972
▲ Max Phase	
0	1872536
1	626
2	1210
3	1023
4	3811
▲ #RO5 Violations	
0	1308006
1	324321
2	168152
3	26095
4	845
▲ Molecular Weight	
[4 to 100)	876
[100 to 200)	33777
[200 to 300)	280679
[300 to 400)	660272
[400 to 500)	531197
[500 to 600)	206640
[600 to 700)	68758

CHEMBL3214695
Name: No Data

CHEMBL3545249
Name: GLPG-0555

CHEMBL4116337
Name: No Data

CHEMBL2108374
Name: DUMORELIN

CHEMBL4116520
Name: No Data

CHEMBL4117176
Name: No Data

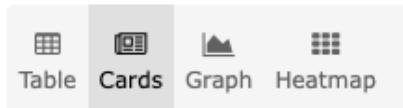
CHEMBL3040331
Name: No Data

CHEMBL3990718
Name: No Data

機能の説明

表示切り替え

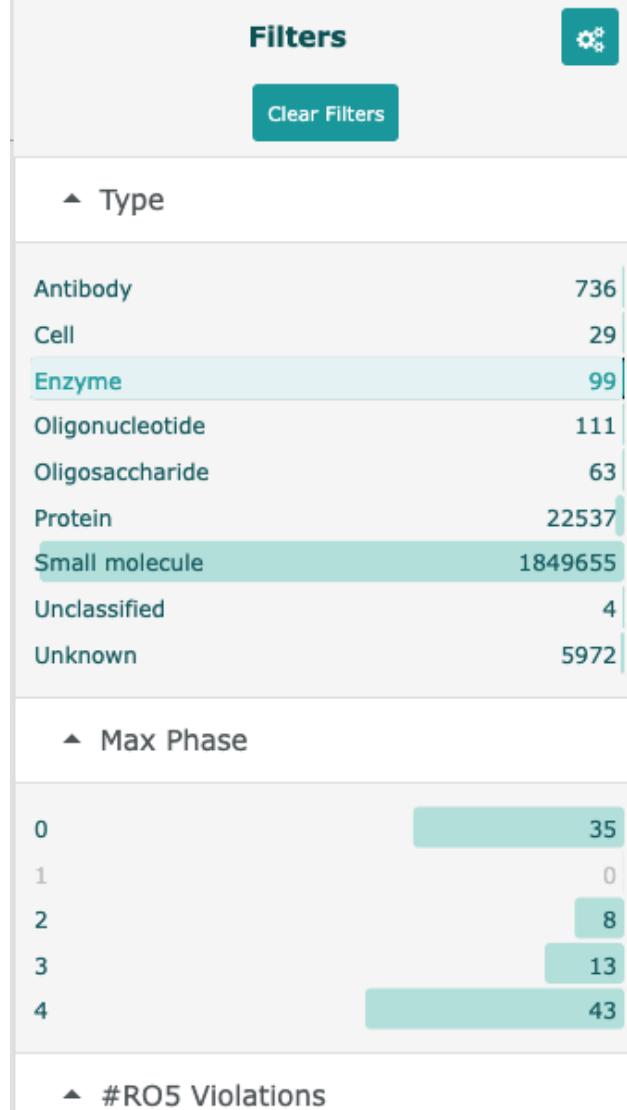
- 左上のTable, Card, Graph, Heatmapをクリックすると表示を切り替えることができます。



絞り込み

- Filterから絞りたい項目をクリックして選択すると、データを絞り込むことができます。

Filters	
▼ Type	
▼ Max Phase	
▼ #RO5 Violations	
▼ Molecular Weight	
▼ AlogP	
▼ Is Drug	
▼ ATC Class. Level 1	
▼ ATC Class. Level 2	
▼ Targets	
▼ Bioactivities	



- [Clear Filters](#) で、フィルターをクリアすることができます。

データダウンロード

- 右上のアイコンからダウンロードする形式を選んで選択したデータをダウンロードすることができます。



EBI > Databases > Chemical Biology > ChEMBL Database > Compounds > Query

Browse Compounds

[Edit Querystring](#)

[Show Full Query](#)

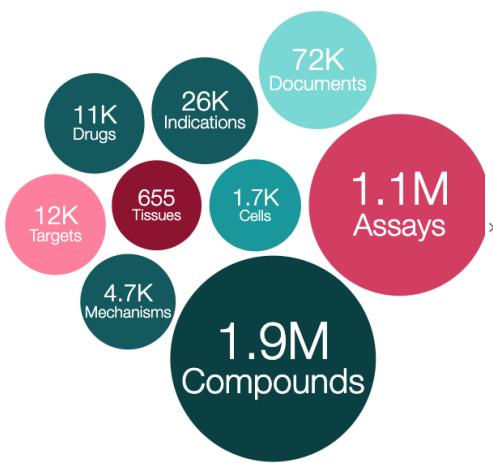
1,879,206 Compounds
0 Selected - Select All
[Browse Activities](#)

Records per page: 20

Showing 1-20 out of 1,879,206 records

ChEMBL ID	Name	Synonyms	Type	Max Phase	Molecular Weight	Targets	Bioactivities	AlogP	PSA	HBA
CHEMBL3214695	No Data	Unknown	0	No Data	0	No data.	No Data	No Data	No Data	No Data
CHEMBL3545249	GLPG-0555	GLPG-0555	Small molecule	1	No Data	0	No Data	No Data	No Data	No Data
CHEMBL4116337	-O-O-O-	No Data	Small molecule	0	524.45	0	No Data	5.27	116.95	7
CHEMBL2108374	DUMORELIN	Dumorelin	Protein	0	No Data	0	No Data	No Data	No Data	No Data
CHEMBL4116520	No Data	Small molecule	0	360.87	0	No data.	No Data	4.3	68.16	4

アッセイ



- 上図の"Assays"をクリックすると、下図のようなアッセイリストが表示されます。

Browse Assays

[Edit Querystring](#)
[Show Full Query](#)

1,125,387 Assays
0 Selected - Select All
[Browse Activities](#)

Records per page: 20 [Show/Hide Columns](#) Showing 1-20 out of 1,125,387 records [1](#) [2](#) [3](#) [4](#) [5](#) ... [CSV](#) [TSV](#)

ChEMBL ID	Description	Organism	Compounds	Document	BAO Format	Source
CHEMBL3214936	PubChem BioAssay. Quorum CqsS/ LuxQ: Assay for inducers of light production in the absence of autoinducers using DH231 (delta cqsS) Measured in Microorganism System Using Plate Reader - 2132-04_Agonist_Dose_DryPowder_Activity_Set2. (absACm _n = the concentration at which the curve crosses threshold nn uM) [Class of assay: confirmatory]	No Data	No Data	CHEMBL1201862	organism-based format	PubChem BioAssays
CHEMBL3214942	PubChem BioAssay. ATP level determination counterscreen in the absence of simvastatin Measured in Cell-Based System Using Plate Reader - 2112-02_Other_Dose_DryPowder_Activity. (absACm _n = the concentration at which the curve crosses threshold nn uM) [Class of assay: confirmatory]	No Data	No Data	CHEMBL1201862	cell-based format	PubChem BioAssays
CHEMBL3215052	PubChem BioAssay. Quorum LuxQ: Assay for inducers of light production in the absence of autoinducers using BH1651 (luxQ047E) Measured in Microorganism System Using Plate Reader - 2132-03_Agonist_Dose_DryPowder_Activity_Set3. (absACm _n = the concentration at which the curve crosses threshold nn uM) [Class of assay: confirmatory]	No Data	No Data	CHEMBL1201862	organism-based format	PubChem BioAssays
CHEMBL3215054	PubChem BioAssay. HTS to identify Pax4 expression activator Measured in Cell-Based System Using RT-PCR - 7144-01_Activator_Dose_CherryPick_Activity. (Class of assay: confirmatory)	No Data	No Data	CHEMBL1201862	cell-based format	PubChem BioAssays

PubChem BioAssay. SNB19 HRAS Target ID Apoptosis Multiple Timepoints

● 左にある”Filters”で、各種条件でフィルターすることができます。

[EBI > Databases > Chemical Biology > ChEMBL Database > Assays > Query](#)

Browse Assays

[Edit Querystring](#)
[Show Full Query](#)

760,843 Assays
0 Selected - Select All
[Browse Activities](#)

Records per page: 20 [Show/Hide Columns](#) Showing 1-20 out of 760,843 records [1](#) [2](#) [3](#) [4](#) [5](#) ... [CSV](#) [TSV](#)

ChEMBL ID	Description	Organism	Compounds	Document	BAO Format	Source
CHEMBL2114806	PubChem BioAssay. Counter screen for HTS for Beta-2AR agonists with FAP-tagged mouse CCR5 with Powerset1. [Class of assay: confirmatory]	Mus musculus	No Data	CHEMBL1201862	assay format	PubChem BioAssays
CHEMBL1613979	PUBCHEM_BIOASSAY: qHTS Assay for Inhibitors and Activators of N3705 glucocerebrosidase as a Potential Chaperone Treatment of Gaucher Disease: Alpha-Galactosidase Counterscreen. [Class of assay: confirmatory] [Related pubchem assays: 2101]	Homo sapiens	No Data	CHEMBL1201862	assay format	PubChem BioAssays
CHEMBL843747	No Data	Rattus norvegicus	No Data	CHEMBL1130110	organism-based format	Scientific Literature
CHEMBL1794448	PUBCHEM_BIOASSAY: PrP Counter Screen: GFP reporter Measured in Cell-Based System Using Imaging - 2078-06_Inhibitor_Dose_DryPowder_Activity. [Class of assay: confirmatory] [Related pubchem assays (depositor defined): AID488894]	Homo sapiens	No Data	CHEMBL1201862	cell-based format	PubChem BioAssays
CHEMBL1738587	PUBCHEM_BIOASSAY: Inhibitors of 12-hLO (12-human lipoxigenase): 15hLO-1 Cuvette-Based Activation Counterscreen Assay for 12hLO Follow up Compounds. [Class of assay: confirmatory] [Related pubchem assays (depositor defined): AID1452, AID2162, AID2163, AID2164, AID2584]	Homo sapiens	No Data	CHEMBL1201862	assay format	PubChem BioAssays
CHEMBL1614180	PUBCHEM_BIOASSAY: Cuvette-Based Assay for Inhibitors of 15-hLO-2 (15-human lipoxigenase 2). [Class of assay: confirmatory] [Related pubchem assays (depositor defined): AID2312, AID2537, AID881]	Homo sapiens	No Data	CHEMBL1201862	assay format	PubChem BioAssays
CHEMBL3885752	The A2A-Star2 receptor has been purified from membranes in n-decyl-beta-D-maltoside as detergent. Ligands were prepared over a five-fold concentration series and injected in either a multi- or a single-cycle format depending on the kinetics parameters of the ligand. The actual concentrations as well as contact and dissociation times varied between the ligands depended on the kinetics and affinity of the interaction. The data were fitted to a 1:1 interaction model using the kinetics evaluation software from Biacore.	Homo sapiens	No Data	CHEMBL3885741	assay format	K4DD Project

● リストにある”ChEMBL ID”的リンクをクリックすると下図のような”Assay Report Card”が表示されます。

- Assay Report Cardには、Basic Information, Curation Summary, Activity Charts, Compound Summaryが含まれています。

Assay Report Card

Basic Information
Curation Summary
Activity Charts
Compound Summary

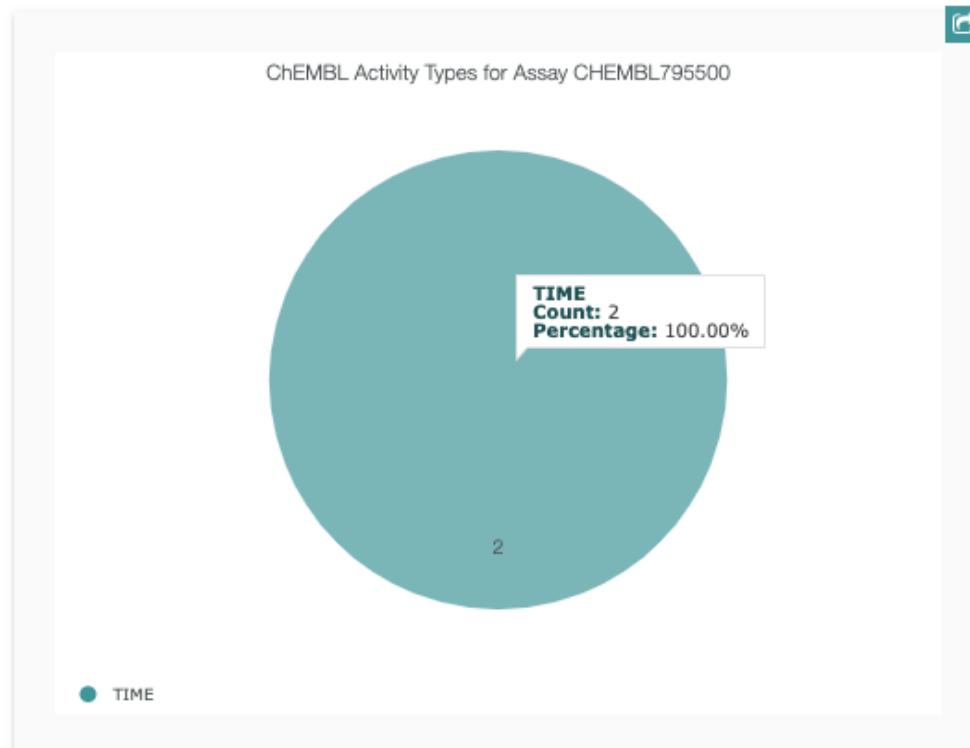
Basic Information

Assay ID:	CHEMBL1815337
Type:	ADME
Description:	Toxicity in male Wistar rat assessed as hemoglobin level at 3 mg/kg, po measured after 28 days (Rvb = 13.66 +/- 0.23 g/dl)
Format:	BAO_0000218
Journal:	Bioorg. Med. Chem. Lett. (2011) 21:3103-3109
Organism:	Rattus norvegicus
Strain:	Wistar
Tissue:	---
Cell Type:	---
Subcellular Fraction:	---
Target:	CHEMBL376
Document:	CHEMBL1811848
Cell:	
Tissue:	

Curation Summary

Target	Target Type	Target Description
Rattus norvegicus (CHEMBL376)	ORGANISM	

Bioactivity



- Bioactivityでクリックすると、活性情報のリストが表示されます。

Browse Activities

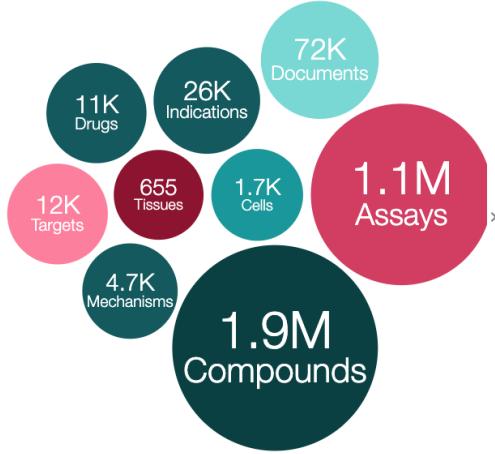
Edit Querystring ⓘ Show Full Query ⓘ

2 Activities
0 Selected - Select All
Browse Compounds ⓘ

CSV TSV

Filters													
Records per page: 20 Show/Hide Columns													
Molecule	Standard Type	Standard Relation	Standard Value	Standard Units	pChEMBL Value	Comment	Compound Key	Assay	Assay Description	BAO Format	Target	Target Pref. Name	Target Organ
 CHEMBL294239	TIME	=	0.008889	hr	No Data	No Data	44 (Enantiomer of 26)	CHEMBL795500	Time for Mean burst suppression ratio (BSR) after the start of a 10 s iv bolus injection of compound	organism-based format	CHEMBL376	Rattus norvegicus	Rattus norveg
 CHEMBL526	TIME	=	0.008333	hr	No Data	No Data	1 (Propofol)	CHEMBL795500	burst suppression ratio (BSR) after the start of a 10 s iv bolus injection of compound	organism-based format	CHEMBL376	Rattus norvegicus	Rattus norveg

targets



- "Targets"をクリックすると、下図のようなリストが表示されます。

EBI > Databases > Chemical Biology > ChEMBL Database > Targets > Query

Browse Targets

Edit Querystring ⓘ Show Full Query ⓘ

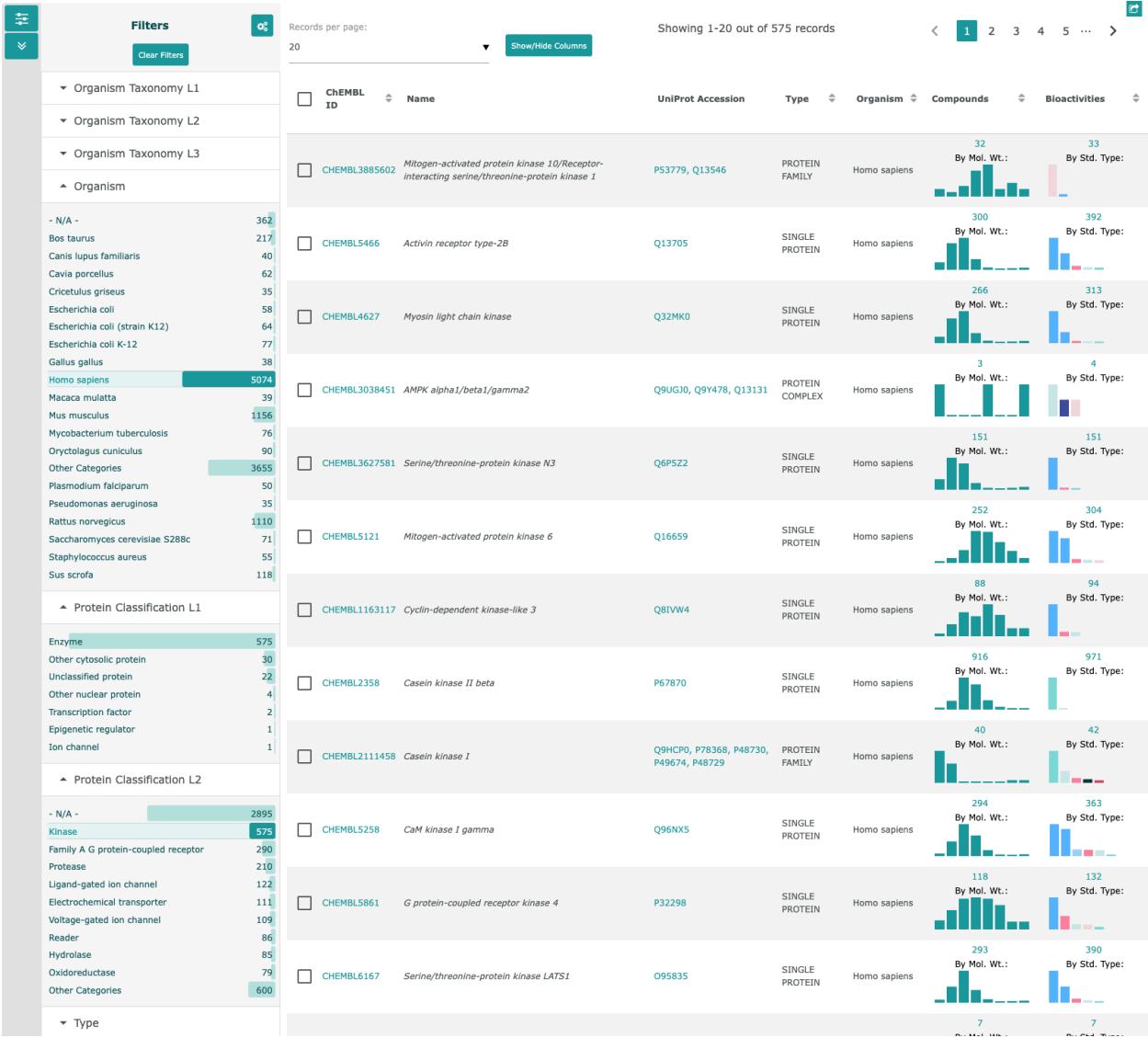
12,482 Targets
0 Selected - Select All
Browse Activities ⓘ

CSV TSV

Filters								
Records per page: 20 Show/Hide Columns								
ChEMBL ID	Name	UniProt Accession	Type	Organism	Compounds	Bioactivities		
CHEMBL3390823	Disialoganglioside GD2		SMALL MOLECULE	Homo sapiens	0 No data.	No Data No data.		
CHEMBL3833503	tRNA		NUCLEIC-ACID	No Data	0 No data.	No Data No data.		
CHEMBL3559389	Triglyceride		LIPID	No Data	0 No data.	No Data No data.		
CHEMBL2366037	Radioactive metals		METAL	No Data	0 No data.	No Data No data.		
CHEMBL2363056	Zinc		METAL	No Data	0 No data.	No Data No data.		
CHEMBL2363058	Iron		METAL	No Data	0 No data.	No Data No data.		
CHEMBL2364029	Lead		METAL	null	0 No data.	No Data No data.		
CHEMBL2366042	DNA		NUCLEIC-ACID	Human herpesvirus 1	0 No data.	No Data No data.		

Organism: Homo Sapiens, Protein Classification L2: Kinase

- 左にあるFiltersを用いて、絞り込むことができます。



- リストの"ChEMBL ID"をクリックすると、下図のような"Target Report Card"が表示されます。

- "Target Report Card"には、以下に示すような様々な情報が含まれています。

EBI > Databases > Chemical Biology > ChEMBL Database > CHEMBL5121

Target Report Card

Name And Classification

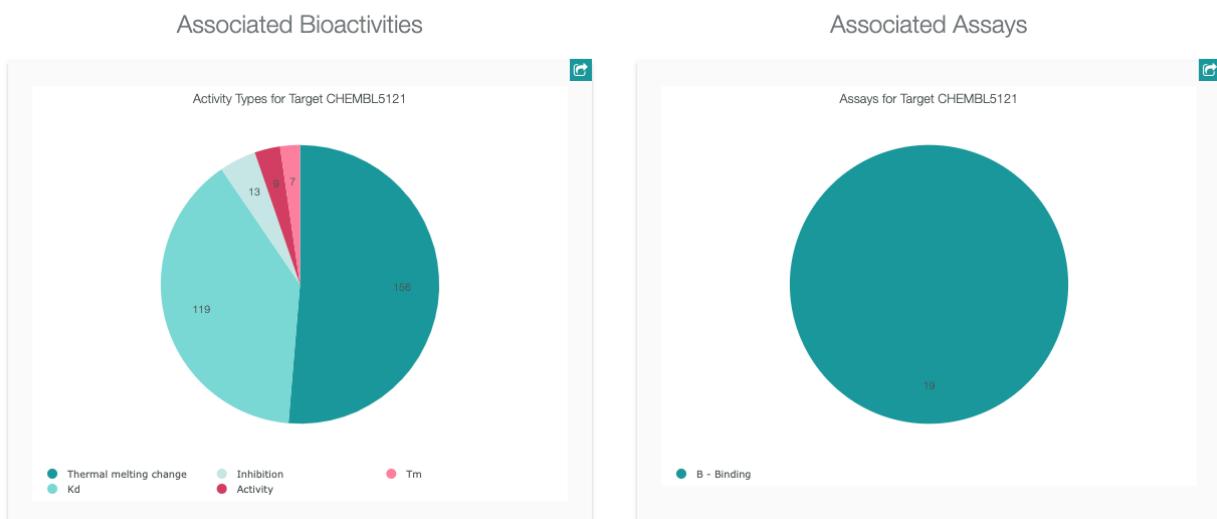
ID:	CHEMBL5121
Type:	SINGLE PROTEIN
Preferred Name:	Mitogen-activated protein kinase 6
Synonyms:	ERK-3 ERK3 Extracellular signal-regulated kinase 3 MAP kinase 6 MAP kinase isoform p97 MAPK p97-MAPK
Organism:	Homo sapiens
Species Group:	No
Protein Target Classification:	- Enzyme > Kinase > Protein Kinase > CMGC protein kinase group > CMGC protein kinase MAPK family > CMGC protein kinase ERK3

Name And Classification
Components
Activity Charts
Ligand Efficiencies
Associated Compounds
Gene Cross References
Protein Cross References
Domain Cross References
Structure Cross References

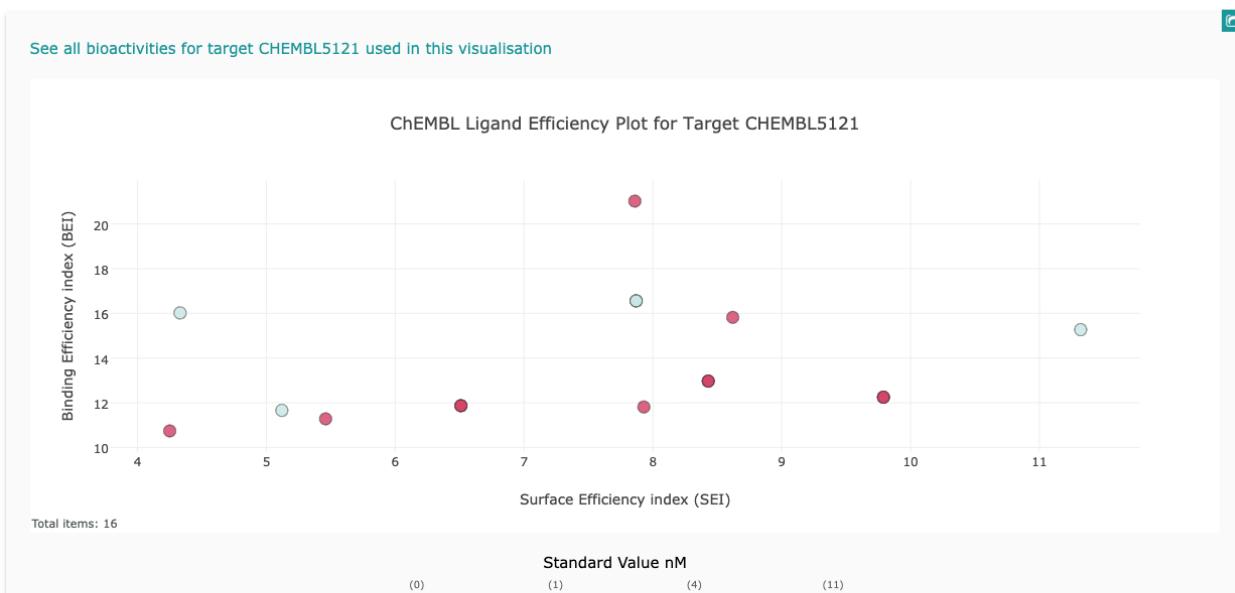
Components

Description	Relationship	Accession
Mitogen-activated protein kinase 6	SINGLE PROTEIN	Q16659

Activity Charts



Ligand Efficiencies



The Ligand Efficiency chart plots Binding Efficiency Index (BEI) against Surface Efficiency Index (SEI), where:

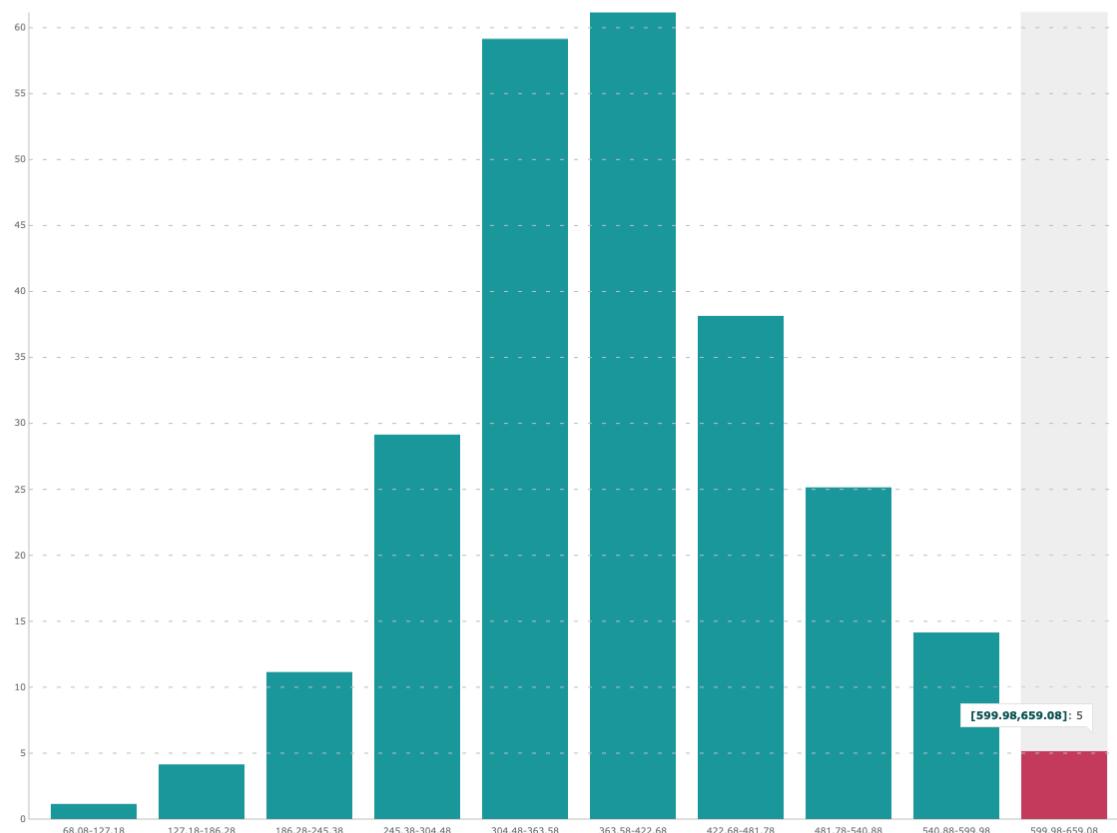
$$\text{SEI} = (-\log_{10}(\text{Standard Value} \cdot 10^{-9})) \cdot 100 / \text{PSA}$$

$$\text{BEI} = (-\log_{10}(\text{Standard Value} \cdot 10^{-9})) \cdot 1000 / \text{MWT}$$

Associated Compounds

X axis:
Parent Molecular WeightNumber of bins: **10**Bin size: **59.1**

Associated Compounds for Target CHEMBL5121 (247)



Gene Cross References

ArrayExpress	ENSG00000069956	
EnsemblGene	ENSG00000069956	
GoComponent	<ul style="list-style-type: none"> GO:0005634 (nucleus) GO:0005654 (nucleoplasm) GO:0005737 (cytoplasm) GO:0005829 (cytosol) GO:0032156 (septin cytoskeleton) GO:0032991 (protein-containing complex) 	
GoFunction	<ul style="list-style-type: none"> GO:0000166 (nucleotide binding) GO:0004672 (protein kinase activity) GO:0004674 (protein serine/threonine kinase activity) GO:0004707 (MAP kinase activity) GO:0005515 (protein binding) GO:0005524 (ATP binding) GO:0016301 (kinase activity) GO:0016740 (transferase activity) GO:0019901 (protein kinase binding) GO:0046982 (protein heterodimerization activity) 	
GoProcess	<ul style="list-style-type: none"> GO:0000165 (MAPK cascade) GO:0006468 (protein phosphorylation) GO:0007049 (cell cycle) GO:0007165 (signal transduction) GO:0010468 (regulation of gene expression) GO:0016310 (phosphorylation) GO:0035556 (intracellular signal transduction) GO:0060999 (positive regulation of dendritic spine development) GO:0071310 (cellular response to organic substance) 	
Wikipedia	MAPK6	

Protein Cross References

canSAR-Target	Q16659	
Human Protein Atlas	ENSG00000069956	
IntAct	Q16659	
Open Targets	ENSG00000069956	
PharmGKB	mitogen-activated protein kinase 6	
Pharos	Tbio	
Reactome	MAPK6/MAPK4 signaling.	
UniProt	B2R945, B5BU65, Q16659, Q68DH4, Q8IYN8	

Domain Cross References

InterPro	<ul style="list-style-type: none"> IPR000719 (Prot_kinase_dom.) IPR008271 (Ser/Thr_kinase_AS.) IPR008350 (MAPK_ERK3/4.) IPR011009 (Kinase-like_dom_sf.) IPR017441 (Protein_kinase_ATP_BS.) 	
Pfam	<ul style="list-style-type: none"> PF00069 (Pkinase) 	

Structure Cross References

The screenshot shows a search results page with two entries:

- CREDO**: ID 2I6L
- PDBe**: ID 2I6L

キーワード検索

化合物・医薬品

レキサルティ

https://www.kegg.jp/medicus-bin/japic_med?japic_code=00067274

医療用医薬品：レキサルティ

[List](#) [Top](#)[添付文書情報](#)[商品詳細情報](#)

医薬品情報

総称名	レキサルティ
一般名	ブレクスピプラゾール
欧文一般名	Brexpiprazole
製剤名	ブレクスピプラゾール錠
薬効分類名	抗精神病薬
薬効分類番号	1179
ATCコード	N05AX16
KEGG DRUG	D10309 ブレクスピプラゾール 商品一覧 米国の商品 相互作用情報
JAPIC	添付文書(PDF)

この情報は KEGG データベース
により提供されています。
日米の医薬品添付文書は[こちら](#)
から検索することができます。

“Brexpiprazole”を検索してみましょう

- トップページ右上の入力欄にキーワードを入力します。今回は“Brexpiprazole”

The search results for "Brexpiprazole" show the following information:

- Search term: Brexpiprazole
- Search results: Search for "Brexpiprazole" in all Compounds
- Result count: BREXPRAZOLE
- Link: Go to Compound CHEMBL2105760

- キーワードを入力すると関連情報が表示されます。ここでは、

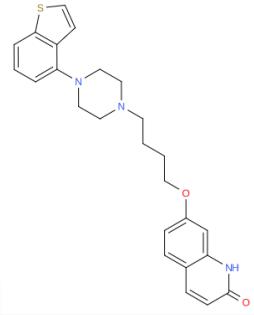
[Search for "Brexpiprazole" in all Compounds](#)

からCompoundsに含まれているデータであることがわかります。

右下に表示される [Go to Compound CHEMBL2105760](#) をクリックすると分子の詳細ページが表示されます。
https://www.ebi.ac.uk/chembl/compound_report_card/CHEMBL2105760/

Compound Report Card

Name And Classification



ID: CHEMBL2105760
Name: BREXPPIRAZOLE
Max Phase: 4 Approved ⓘ
Molecular Formula: C₂₉H₂₇N₃O₂S
Molecular Weight: 433.58
ChEMBL Synonyms: BREXPPIRAZOLE, OPC-34712
Trade Names: REXULTI
Molecule Type: Small molecule

Name And Classification
 Representations
 Sources
 Molecule Features
 Mechanism Of Action
 Indications
 Clinical Data
 Similar Compounds
 Activity Charts
 Literature
 Target Predictions
 Calculated Properties
 Structural Alerts
 Cross References
 UniChem Cross References
 UniChem Connectivity Layer Cross References
 References
 Alternative Forms

Representations

Molfile:

</>
View Raw
Download
Editor
Copy

Canonical SMILES: O=C1Nc2cc(OCCCCN3CCN(CC3)C4CCCC5SCCC45)ccc2C=C1

Standard InChI: InChI=1S/C25H27N3O2S/c29-25-9-7-19-6-8-28(18-22(19)26-25)30-16-2-1-11-27-12-14-28(15-13-27)23-4-3-5-24-21(23)10-17-31-24/h3-10,17-18H,1

Standard InChI Key: ZKIAIYBUSXZPLP-UHFFFAOYSA-N

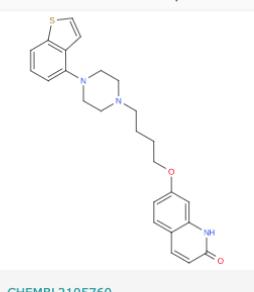
Sources

Sources:

BindingDB Database Orange Book USP Dictionary of USAN and International Drug Names WHO Anatomical Therapeutic Chemical Classification

Alternative Forms

Alternative forms of compound CHEMBL2105760 (Parent):



CHEMBL2105760

Molecule Features















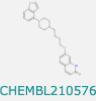
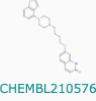
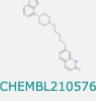






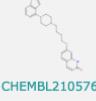
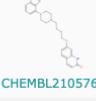
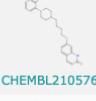
Mechanism Of Action

Records per page: 20 [Browse All](#)

Molecule CHEMBL ID	Molecule Name	Molecule Type	Max Phase	First Approval	USAN Stem	Mechanism Of Action	Target CHEMBL ID	Target Name	Mechanism Type	Target Type	Target Organism
 CHEMBL2105760	BREXPIRAZOLE	Small molecule	4	2015	-prazole	Serotonin 2a (5-HT2a) receptor antagonist	CHEMBL224	Serotonin 2a (5-HT2a) receptor	ANTAGONIST	SINGLE PROTEIN	Homo sapiens
 CHEMBL2105760	BREXPIRAZOLE	Small molecule	4	2015	-prazole	Dopamine D2 receptor partial agonist	CHEMBL217	Dopamine D2 receptor	PARTIAL AGONIST	SINGLE PROTEIN	Homo sapiens
 CHEMBL2105760	BREXPIRAZOLE	Small molecule	4	2015	-prazole	Serotonin 1a (5-HT1a) receptor partial agonist	CHEMBL214	Serotonin 1a (5-HT1a) receptor	PARTIAL AGONIST	SINGLE PROTEIN	Homo sapiens

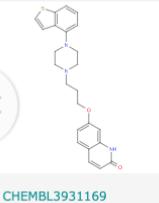
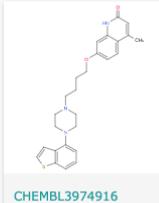
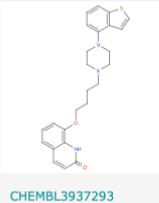
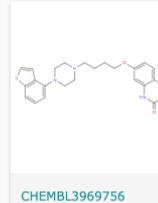
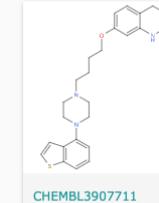
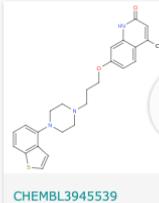
Indications

Records per page: 20 [Browse All](#)

ChEMBL ID	Molecule Name	Molecule Type	Max Phase for Indication	First Approval	MESH ID	MESH Heading	EFO ID	EFO Term	Indication References
 CHEMBL2105760	BREXPIRAZOLE	Small molecule	3	2015	D003866	Depressive Disorder	EFO:0003761	unipolar depression	ClinicalTrials
 CHEMBL2105760	BREXPIRAZOLE	Small molecule	3	2015	D007319	Sleep Initiation and Maintenance Disorders	EFO:0004698	insomnia	ClinicalTrials
 CHEMBL2105760	BREXPIRAZOLE	Small molecule	4	2015	D003865	Depressive Disorder, Major	EFO:0003761	unipolar depression	DailyMed

Similar Compounds

Compounds similar to CHEMBL2105760 with at least 85% similarity, see [full list](#):

 CHEMBL3931169	 CHEMBL3974916	 CHEMBL3937293	 CHEMBL3969756	 CHEMBL3907711	 CHEMBL3945539
---	---	---	---	---	---

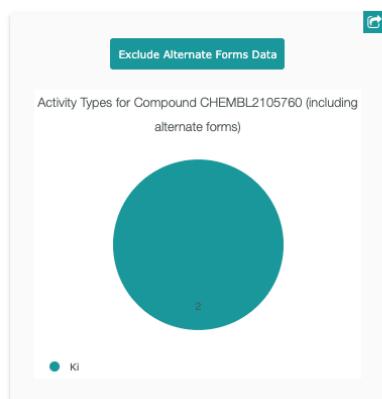
Showing 1-6 out of 26 records

1 2 3 4 5

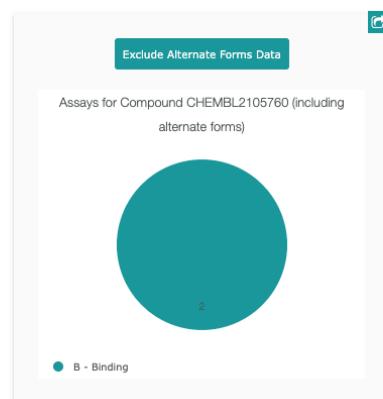
Activity Charts



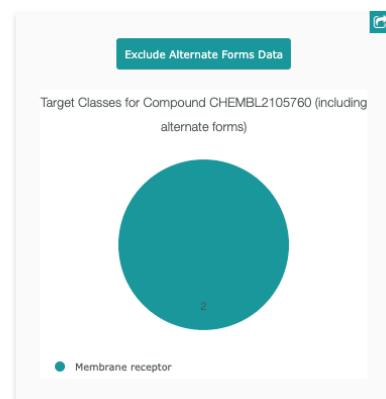
Bioactivity Summary



Assay Summary



Target Summary



Target Predictions



The two tables below display ChEMBL single-protein targets which are predicted to interact with CHEMBL25. A 1uM and 10 uM cut-off have been applied to ChEMBL bioactivity data used to generate the respective models and the green coloured rows correspond to genuine predictions, i.e. targets not included in the original training set for this compound.

1uM

Records per page:

5



Target	Target Pref. Name	Organism	Score	In Training Set
CHEMBL322	No Data	Rattus norvegicus	1.000	yes
CHEMBL339	No Data	Rattus norvegicus	1.000	yes
CHEMBL214	No Data	Homo sapiens	1.000	no
CHEMBL217	No Data	Homo sapiens	1.000	no
CHEMBL273	No Data	Rattus norvegicus	1.000	no

Showing 1-5 out of 50 records

< 1 2 3 4 5 ... >

10uM

Records per page:

5



Target	Target Pref. Name	Organism	Score	In Training Set
CHEMBL322	No Data	Rattus norvegicus	1.000	yes
CHEMBL339	No Data	Rattus norvegicus	1.000	yes
CHEMBL214	No Data	Homo sapiens	1.000	no
CHEMBL273	No Data	Rattus norvegicus	1.000	no
CHEMBL217	No Data	Homo sapiens	1.000	no

Showing 1-5 out of 50 records

< 1 2 3 4 5 ... >

Calculated Properties

Mol. Weight:	433.58
MW. Monoisotopic:	433.1824
ALogP:	4.72
#Rotatable Bonds:	7
Polar Surface Area:	48.57
Molecular Species:	NEUTRAL
HBA:	5
HDB:	1
#Ro5 Violations:	0
HBA (Lipinski):	5
HBD (Lipinski):	1
#Ro5 Violations (Lipinski):	0
ACD Acidic pKa:	11.22
ACD Basic pKa:	--
#ACD LogP:	3.41
ACD LogD pH7.4:	--
Aromatic Rings:	4
Heavy Atoms:	31
QED Weighted:	0.43

Cross References

	N - NERVOUS SYSTEM N05 - PSYCHOLEPTICS N05A - ANTIPSYCHOTICS N05AX - Other antipsychotics N05AX16 - brexpiprazole
ChemSpider	ChemSpider:ZKIAIYBUSXZPLP-UHFFFAOYSA-N
DailyMed	brexpiprazole

UniChem Cross References



BindingDB	194780
ChEBI	134716
ChemicalBook	CB52681994
DrugBank	DB09128
DrugCentral	5014
EPA CompTox Dashboard	DTXSID40238527
FDA SRS	2J3YBM1K8C
Guide to Pharmacology	7672
IBM Patent System	4E1CCBE9842C219666EF027598E5FA30
LINCS	LSM-45790
MolPort	MolPort-046-033-502, MolPort-039-063-477
Nikkaji	J3.002.326I
PharmGKB	PA166160053
PubChem	11978813
PubChem: Thomson Pharma	17430973
SureChEMBL	SCHEMBL1037592
ZINC	ZINC000084758479

UniChem Connectivity Layer Cross References



UniChem Connectivity Layer Cross References for CHEMBL2105760



ZKIAIYBUSXZPLP-UHFFFAOYSA-N

Full InChI:

InChI=1S/C25H27N3O2S/c29-25-9-7-19-6-8-20(18-22(19)26-25)30-16-2-1-11-27-1 ... 5-13-27)23-4-3-5-24-21(23)10-17-31-24/h3-10,17-18H,1-2,11-16H2,(H,26,29)



Columns Legend:

S = stereochemical difference.

I = isotopic difference.

P = protonation differences identified.

Include Alternative Salts and Mixtures

Records per page:

5



Source	Identical Component	S	I	P	SI	IP	SP	SIP
ChEMBL	CHEMBL2105760							
DrugBank	DB09128							
Guide to Pharmacology	7672							
ChEBI	134716							
ZINC	ZINC000084758479							

Showing 1-5 out of 18 records

< 1 2 3 4 >

UniChem REST Service Call: https://www.ebi.ac.uk/unichem/rest/key_search/ZKIAIYBUSXZPLP-UHFFFAOYSA-N/0/0/4

遺伝子名

- **MAPK6**遺伝子
ヒトでマイトジエン活性化プロテインキナーゼ6をコードするMAPK6遺伝子

MAPK6

Search for "MAPK6" in all Targets

MAPK6

Go to Target CHEMBL5121

Search for "MAPK6" in all Targets

からTargetsに含まれていることがわかります。

右下に表示される [Go to Target CHEMBL5121](#) をクリックすると [詳細ページ](#)へ移動します。

EBI > Databases > Chemical Biology > ChEMBL Database > CHEMBL5121

Target Report Card

Name And Classification

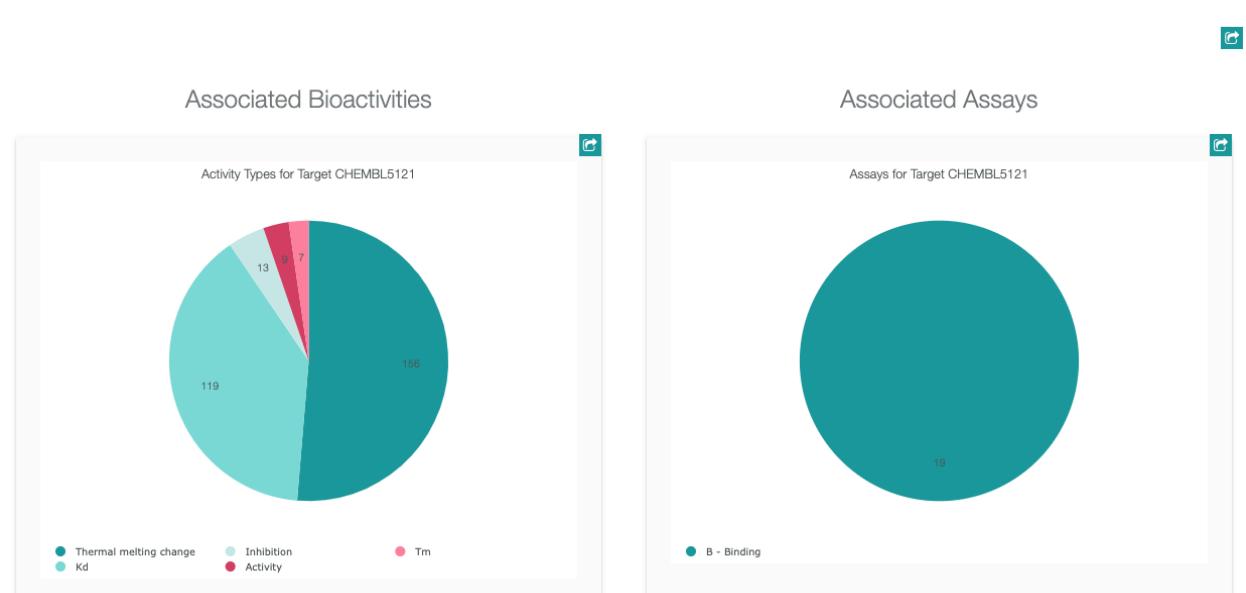
ID:	CHEMBL5121
Type:	SINGLE PROTEIN
Preferred Name:	Mitogen-activated protein kinase 6
Synonyms:	ERK-3 ERK3 Extracellular signal-regulated kinase 3 MAP kinase 6 MAP kinase isoform p97 MAPK 6 MAPK6 Mitogen-activated protein kinase 6 PRKM6 p97-MAPK
Organism:	Homo sapiens
Species Group:	No
Protein Target Classification:	- Enzyme > Kinase > Protein Kinase > CMGC protein kinase group > CMGC protein kinase MAPK family > CMGC protein kinase ERK3

Name And Classification
Components
Activity Charts
Ligand Efficiencies
Associated Compounds
Gene Cross References
Protein Cross References
Domain Cross References
Structure Cross References

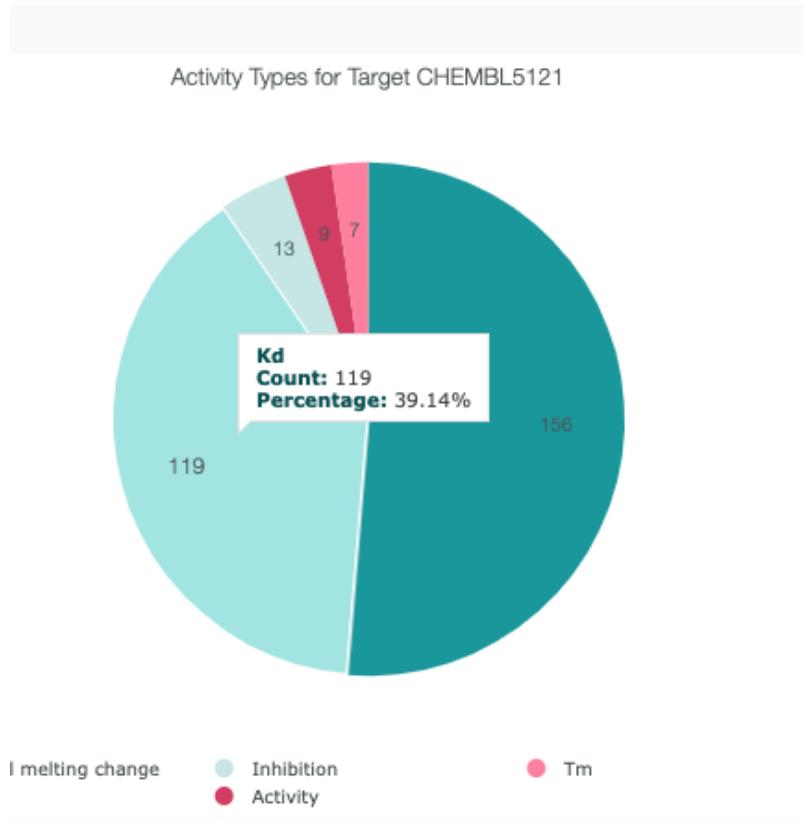
Components

Description	Relationship	Accession
Mitogen-activated protein kinase 6	SINGLE PROTEIN	Q16659

Activity Charts



Associated Bioactivities



EBI > Databases > Chemical Biology > ChEMBL Database > Activities > Query

Browse Activities

[Edit Querystring](#) [Show Full Query](#)

119 Activities
0 Selected - Select All [Browse Compounds](#)

CSV TSV

Records per page: 20 Show/Hide Columns

Showing 1-20 out of 119 records

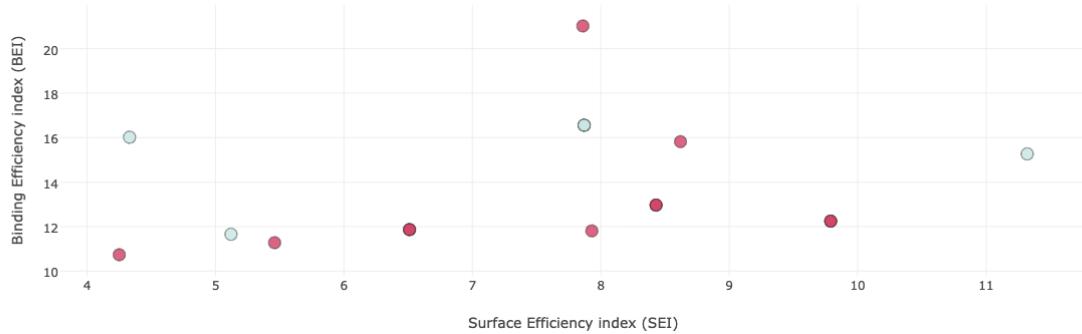
Molecule	Standard Type	Standard Relation	Standard Value	Standard Units	pChEMBL Value	Comment	Compound Key	Assay	Assay Description	BAO Format
	Kd	>	10000	nM	No Data	No Data	GSK-1838705A	CHEMBL1908584	Binding constant for ERK3 kinase domain	single protein format
	Kd	>	10000	nM	No Data	No Data	AB-1010	CHEMBL1908584	Binding constant for ERK3 kinase domain	single protein format
	Kd	=	1700	nM	5.77	No Data	CI-1033	CHEMBL1908584	Binding constant for ERK3 kinase domain	single protein format
	Kd	>	10000	nM	No Data	No Data	PTK-787	CHEMBL1908584	Binding constant for ERK3 kinase domain	single protein format

Ligand Efficiencies



See all bioactivities for target CHEMBL5121 used in this visualisation

ChEMBL Ligand Efficiency Plot for Target CHEMBL5121



The Ligand Efficiency chart plots Binding Efficiency Index (BEI) against Surface Efficiency Index (SEI), where:

$$\text{SEI} = (-\log_{10}(\text{Standard Value} \times 10^{-9})) \times 100 / \text{PSA}$$

$$\text{BEI} = (-\log_{10}(\text{Standard Value} \times 10^{-9})) \times 1000 / \text{MWt}$$

- 各プロットにマウスカーソルをのせると、プロットの情報が表示されます。

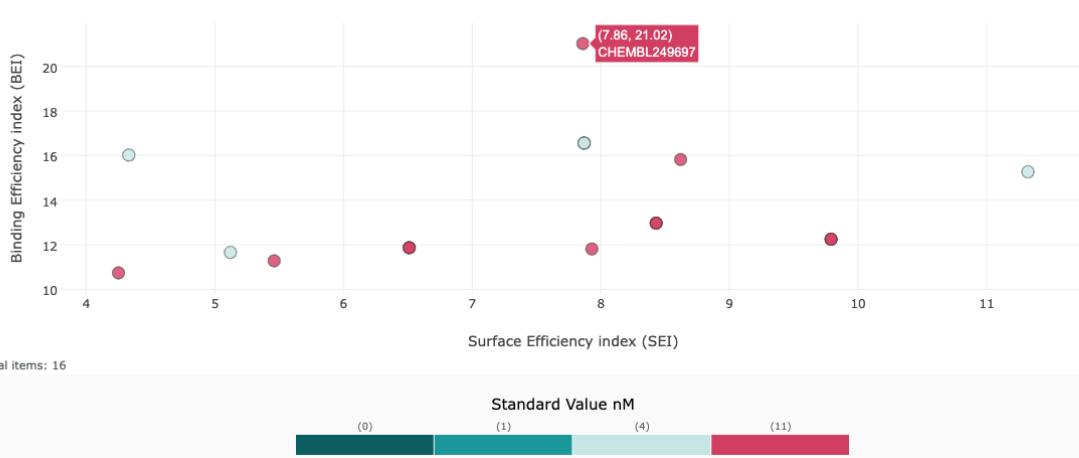
BEI / Binding Efficiency Index / 結合効率指数
SEI / Surface-binding Efficiency Index / 表面結合効率指数

Ligand Efficiencies



See all bioactivities for target CHEMBL5121 used in this visualisation

ChEMBL Ligand Efficiency Plot for Target CHEMBL5121

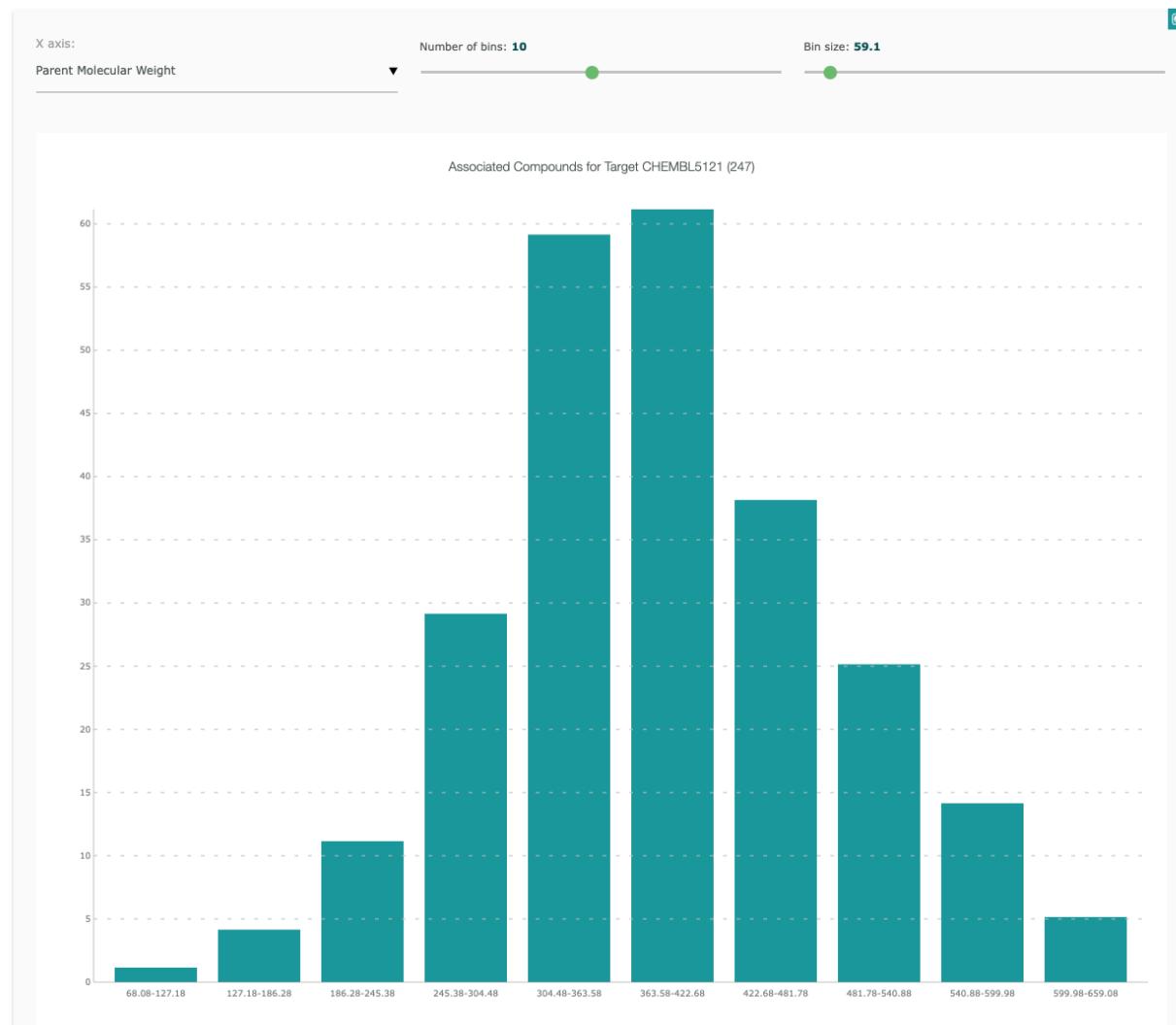


The Ligand Efficiency chart plots Binding Efficiency Index (BEI) against Surface Efficiency Index (SEI), where:

$$\text{SEI} = (-\log_{10}(\text{Standard Value} \times 10^{-9})) \times 100 / \text{PSA}$$

$$\text{BEI} = (-\log_{10}(\text{Standard Value} \times 10^{-9})) \times 1000 / \text{MWt}$$

Associated Compounds



Gene Cross References

	
ArrayExpress	ENSG00000069956
EnsemblGene	ENSG00000069956
GoComponent	<ul style="list-style-type: none"> GO:0005634 (nucleus) GO:0005654 (nucleoplasm) GO:0005737 (cytoplasm) GO:0005829 (cytosol) GO:0032156 (septin cytoskeleton) GO:0032991 (protein-containing complex)
GoFunction	<ul style="list-style-type: none"> GO:0000166 (nucleotide binding) GO:0004672 (protein kinase activity) GO:0004674 (protein serine/threonine kinase activity) GO:0004707 (MAP kinase activity) GO:0005515 (protein binding) GO:0005524 (ATP binding) GO:0016301 (kinase activity) GO:0016740 (transferase activity) GO:0019901 (protein kinase binding) GO:0046982 (protein heterodimerization activity)
GoProcess	<ul style="list-style-type: none"> GO:0000165 (MAPK cascade) GO:0006468 (protein phosphorylation) GO:0007049 (cell cycle) GO:0007165 (signal transduction) GO:0010468 (regulation of gene expression) GO:0016310 (phosphorylation) GO:0035556 (intracellular signal transduction) GO:0060999 (positive regulation of dendritic spine development) GO:0071310 (cellular response to organic substance)
Wikipedia	MAPK6

Protein Cross References

	
canSAR-Target	Q16659
Human Protein Atlas	ENSG00000069956
IntAct	Q16659
Open Targets	ENSG00000069956
PharmGKB	mitogen-activated protein kinase 6
Pharos	Tbio
Reactome	MAPK6/MAPK4 signaling.
UniProt	B2R945, B5BU65, Q16659, Q68DH4, Q8IYN8

Domain Cross References

	
InterPro	<ul style="list-style-type: none"> IPR000719 (Prot_kinase_dom.) IPR008271 (Ser/Thr_kinase_AS.) IPR008350 (MAPK_ERK3/4.) IPR011009 (Kinase-like_dom_sf.) IPR017441 (Protein_kinase_ATP_BS.)
Pfam	PF00069 (Pkinase)

Structure Cross References



CREDO	2I6L
PDBe	2I6L

付録：ドキュメント作成手順

1. Google Documentで内容作成
2. Google Documentの”ファイル”→”形式を指定してダウンロード”で、”ウェブページ(html)”を選択する。
3. ダウンロードしたzipファイルを解凍する。
4. HTML - Markdown 変換
 - a. <https://pronama.jp/md/>
5. Githubへhtmlとmdファイル、必要な画像ファイルをアップロード

以上