

LSKB Ver.3.4 Release Note

This document is written New function and fixed bug in LSKB (Life Science Knowledge Bank).

[New Function]

1. Add contents and function at Chemical information

* PDB Ligand Chemical Component

"PDB Ligand Chemical Component" part is added on Chemical information.

In case of the compound which is registered as "Ligand Chemical Component" on PDB, Identifier and compound name are showed, PDB entries equivalent to the compound are listed. Also, LSKB originally mined ligand registered on LSKB compound dictionary. In this case, there is not entry on PDB. It just shows related PDB entry only.

Display on compound information

Ligand ID (Identifier), chemical name on PDB are shown. The number is No. of publication including the name. The list is PDB entries which this ligand registered.

Description of PDB details

Identifier	Name
MT1	<input type="checkbox"/> N-(4-((2,4-DIAMINOPTERIDIN-1-IUM-6-YL)METHYL)(METHYL)AMINO) BENZOYL)-L-GLUTAMIC ACID
PDB Entries 219q Neutron Crystal Structure of Escherichia coli Dihydrofolate Reductase Bound to the Anti-cancer drug, Methotrexate	
Identifier	Name
MTX	<input type="checkbox"/> Methotrexate 21807
PDB Entries	
1ao8	DIHYDROFOLATE REDUCTASE COMPLEXED WITH METHOTREXATE, NMR, 21 STRUCTURES
1axw	E. COLI THYMIDYLATE SYNTHASE IN COMPLEX WITH METHOTREXATE (MTX) AND 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (DUMP)
1d1a	DIHYDROFOLATE REDUCTASE FROM THERMOTOGA MARITIMA
1w3d	DIHYDROFOLATE REDUCTASE FROM MYCOBACTERIUM TUBERCULOSIS AND METHOTREXATE
1d1a	EFFECTS IN A SECOND-SITE REVERTANT OF A MUTANT DIHYDROFOLATE REDUCTASE
... more (35)	

Name	Accession
<input type="checkbox"/> Methotrexate	21807 DB00563

Ligand extracted originally from PDB structure by LSKB

No display of Identifier and compound name. It displays PDB entry only.

* Search “related drug” which Metabolizing Enzyme of DrugBank on the compound information.

Drug Target		
Target 1	Target Name	Dihydrofolate reductase
	Target Gene Name	DHFR
	Target SwissProt ID	P00374 > UniProt
	Target Protein	DYR_HUMAN > UniProt >>> Search Related Drugs
	Target PDB ID	1mvt

Phase I Metabolizing Enzyme		
Enzyme 1	Enzyme Name	Aldehyde oxidase
	Enzyme SwissProt ID	Q06278 > UniProt
	Enzyme Protein	ADO_HUMAN > UniProt >>> Search Related Drugs
Enzyme 2	Enzyme Name	Methylenetetrahydrofolate reductase
	Enzyme SwissProt ID	P42

DrugBank Info.

Metabolizing Enzyme
ADO_HUMAN Aldehyde oxidase (1.2.3.1)

11 entries found.

Chemical Name	Count
brimonidine	1281
Chlorpromazine	30426
Famciclovir	987
Methotrexate	22373
NADH	18703
Palonosetron	136
Penciclovir	421
Raloxifene	3160
Vitamin K 3	7760
Zaleplon	241
Zonisamide	713

1 / 1

2. Add Search functions on Protein details Info.

- 1) Search drugs targeting this protein
- 2) Search drugs metabolized by this protein

SwissProt

XDH_HUMAN > UniProt

Primary Accession **P47989**
 Secondary Q16681, Q16712, Q4PJ16
 Protein names Xanthine dehydrogenase/oxidase (1.17.1.4) (1.17.3.2)

>>> [Search drugs targeting this protein](#)
 >>> [Search drugs metabolized by this protein](#)

Gene	Symbol	Gene Name	Evidence
	XDH	xanthine dehydrogenase	by Gene ID by Name

PDB

Check All Clear Download > **BW3DE** Text File Download PDB IDs

PDB ID	Title	Ligand	Source / P
2cki	HUMAN MILI		

Metabolizing Enzyme
 XDH_HUMAN Xanthine dehydrogenase/oxidase (1.17.1.4) (1.17.3.2)

16 entries found.

Chemical Name	Count
alpha-Tocopherol	23795
Carvedilol	2071
Daunorubicin	5423
Deferoxamine	5417
Desflurane	1413
Mercaptopurine	8051
Methotrexate	22373

Download listed structures as spreadsheet on BW3DE

[Send Result to BW3DE](#)

3. New direct linkage to compound information on PDB ligand Identifier (3 character code).

PDB

[PPARG] peroxisome proliferator-activated receptor gamma

CheckAll Clear Download > Text File Download PDB IDs

UniProt Entry Description

[PPARG_HUMAN](#) Peroxisome proliferator-activated receptor gamma (Nuclear receptor subfamily 1 group C member 3)

> [UniProt](#)

PDB ID	Title	Ligand	Source / Resolution
<input type="checkbox"/> 1fm6	THE 2.1 ANGSTROM RESOLUTION CRYSTAL STRUCTURE OF THE HETERODIMER OF THE HUMAN RXRALPHA AND PPARGAMMA LIGAND BINDING DOMAINS RESPECTIVELY BOUND WITH 9-CIS RETINOIC ACID AND ROSIGLITAZONE AND CO-ACTIVATOR PEPTIDES	BRL Refer to Dictionary	Xray 2.1
<input type="checkbox"/> 1fm9	THE 2.1 ANGSTRO THE HETERODIME PPARGAMMA LIG BOUND WITH 9-CI ACTIVATOR PEPT		

BRL PubMed total: 4455

PubChem Compound: [445655_29010895](#)
ZINC: [ZINC00968323](#)

Pharmacological Actions

Chemical Actions and Uses
Pharmacologic Actions
Physiological Effects of Drugs
Hypoglycemic Agents >>> [Search Related Chemicals](#)

3D Viewer Relation Search Check All Clear Send to Clipboard

* Action for CheckBox * Submit

PDB Ligand Chemical Component

Identifier	Name
<input type="checkbox"/> BRL	2,4-THIAZOLIDINEDIONE, 5-[[4-[2-(METHYL-2-PYRIDINYLAMINO) ETHOXY]PHENYL]METHYL]-(9CL)

PDB Entries

1fm6	THE 2.1 ANGSTROM RESOLUTION CRYSTAL STRUCTURE OF THE HETERODIMER OF THE HUMAN RXRALPHA AND PPARGAMMA LIGAND BINDING DOMAINS RESPECTIVELY BOUND WITH 9-CIS RETINOIC ACID AND ROSIGLITAZONE AND CO-ACTIVATOR PEPTIDES.
1zgy	Structural and Biochemical Basis for Selective Repression of the Orphan Nuclear Receptor LXR1 by SREBP

Link in case of "Refer to Dictionary"

NAP	Xray 1.8
CIT	Xray 2.0
Refer to Dictionary	
FID	Xray 2.8
NAP	

Search Keyword: CIT

14 entries found. >>> [Download All](#)

Chemical Name (Product:Name)

<input checked="" type="radio"/> (S)-2-Methylmalate	
<input type="radio"/> CIT	
<input type="radio"/> CIT	
<input type="radio"/> CIT	

Search using query as ligand Identifier

4. Search by Gene ID on top” Gene Synonym Search”

The same display style as previous version.

Enter number as keyword → Gene ID Search ON

Gene Symbol	Gene Name	PF#	More Info
<input type="checkbox"/> PPARG		321	Nucleotide
<input type="checkbox"/>	peroxisome proliferator-activated receptor gamma	2612	Nucleotide
<input type="checkbox"/>	nuclear receptor subfamily 1 group C member 3	-	
<input type="checkbox"/>	peroxisoma proliferativa activatada receptor gamma (PPAR(G)) mRNA	-	Nucleotide

Option display changes to default

5. New search function on Batch search on “Advanced Search”

Keyword type/Search Target	Input value/ Summary of search result
Protein ID	4types of ID and Accession number can be used <ul style="list-style-type: none"> - Accession number of RefSeq Protein - Accession number and entry name of UniProt - Accession number of GenBank Protein
Gene	Gene information related to protein <ul style="list-style-type: none"> - Gene ID - Species - Gene symbol - Gene Name
PDB ID	PDB ID
PDB	Information of PDB Entry <ul style="list-style-type: none"> - PDB ID - Title - Ligand - Experimental Method - Resolution (In case of X-ray)
Protein	UniProt Protein entry information <ul style="list-style-type: none"> - registration Name - Description - Domain (Pfam Accession ID, Description)

Keyword Type : Protein ID

Input Keywords

Text: Q9Y618, NP_002469, P15172, NP_001941, Q16254

File

Keyword Type: Protein ID

Search Target: Gene

Keyword Type : PDB ID

Input Keywords

Text: 1nyx, 1prg, 1rdt, 1wm0, 1zeo

File

Keyword Type: PDB ID

Search Target: PDB