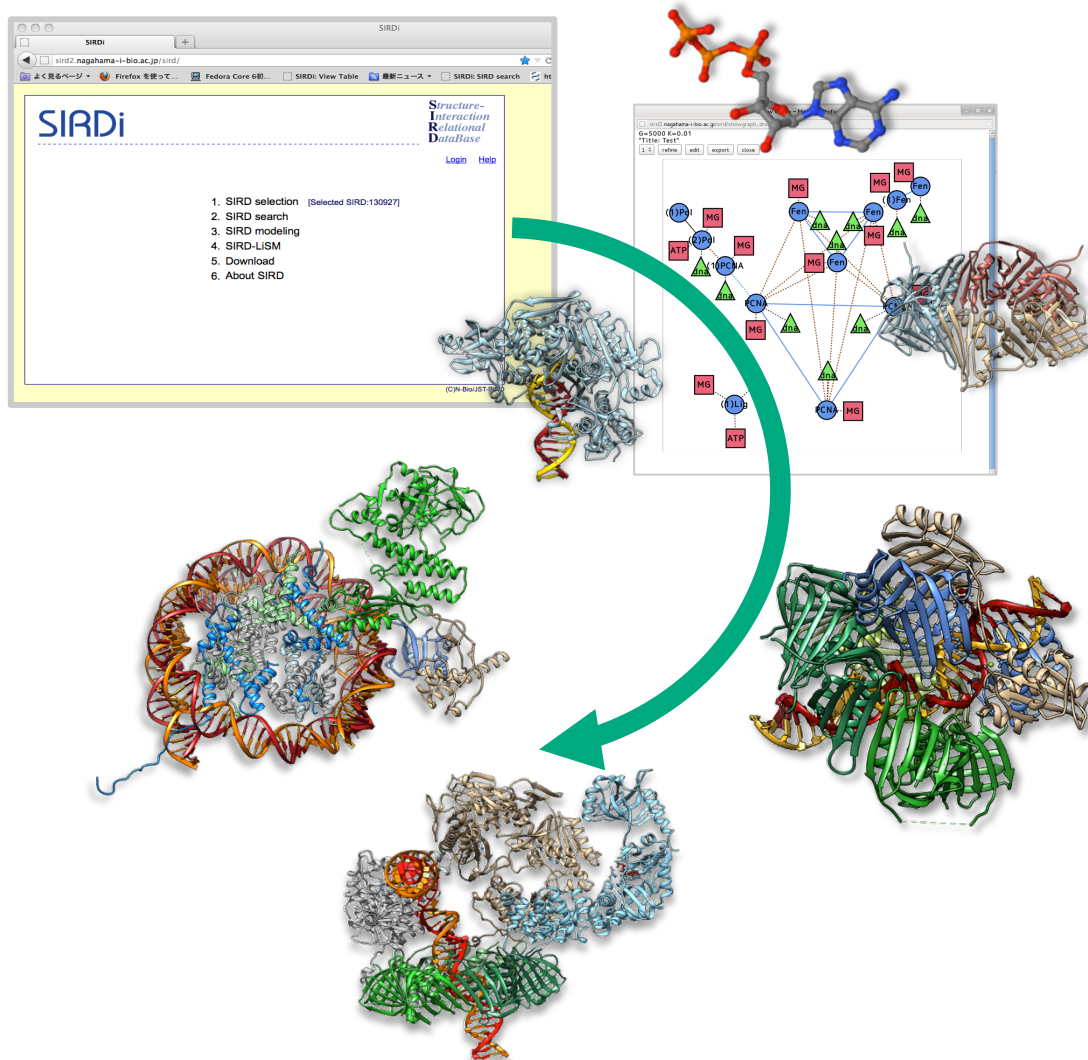
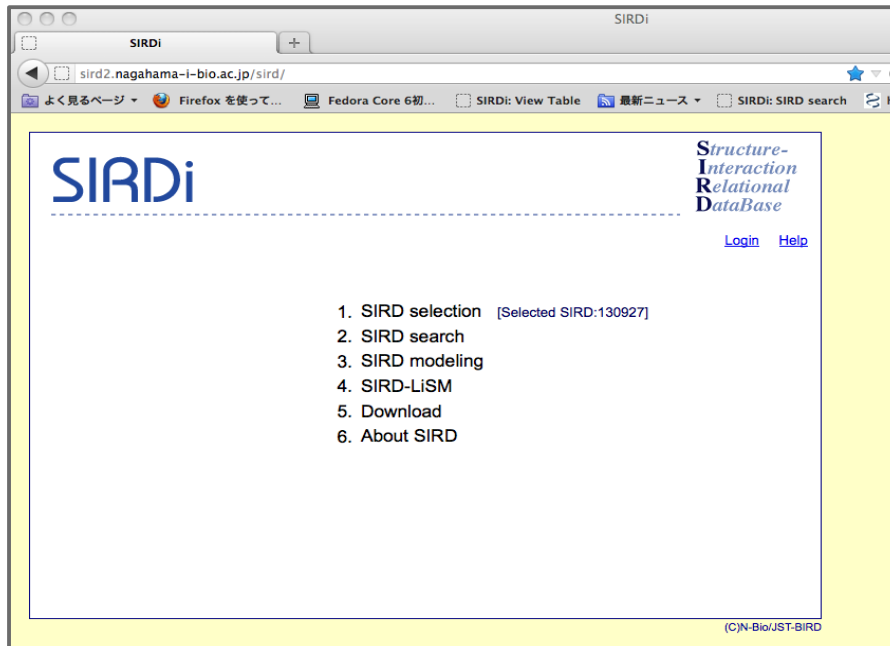


Easy manual for SIRD interface



What is SIRD interface

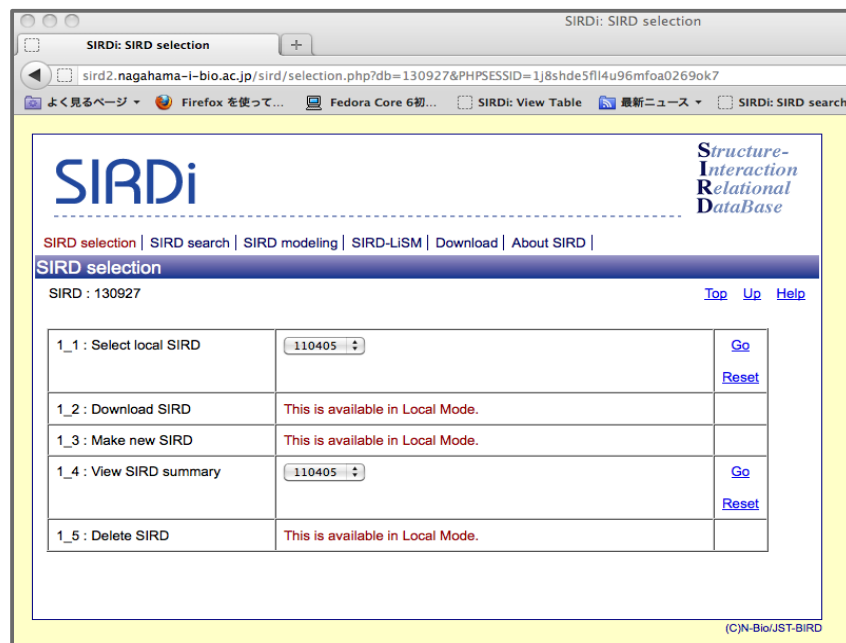
- (1) SIRDi is the web-based interface for SIRD (Structure-Interaction Relational Database)
- (2) You can search for protein structure models with sequence, 3D structure, keyword, ligand, etc.. by using SIRDi



(W1) SIRDi portal

How to select Database

- (1) Click [1. SIRD selection] at portal (W1)
- (2) Choose database version (named after production date YYMMDD) through [1_1: Select local SIRD] and press [Go] (if necessary. Default DB is the latest one)
- (3) Summary for each database can be viewed through [1_4: View SIRD summary]



(W2) DB selection

How to search SIRD database

- (1) Click [2. SIRD search] at portal (W1)
- (2) Fill boxes in [2_1: Select] (W3a) with your search conditions as many as you want (e.g. PDB code for [PDB], Chain ID for [Chain], name of protein for [Name], source organism for [Organism], interacting molecule code for [Ligand], etc...).
- (3) You can name new table by filling [Table Out] box.
- (4) Press [Go] for start search.
- (5) ['table name' is created] will appear on top if table is successfully created (W3b). [ERROR No data for new table] means no data hits your query.

(W3a) Selection window

SIRD : 130927

2.1: Select

☐ Representative ☒ All

Go Reset

PDB	Chain	DomainNo
Name	Organism	
congerin		
Size	Alpha	Beta
3Ddom	3Dsub	1D
LIG	PPI	ANO
ContactID	Ligand	Keyword
	LIGDIC	KWDIC

Table Out: tbl0001

(W3b) Table creation

SIRD selection | SIRD search | SIRD modeling | SIRD-LISM | Download | About SIRD

SIRD : 130927

"tbl0001" is created.

2.1: Select

☐ Representative ☒ All

Go Reset

How to view search results

- (1) Select table in [2_3: View Table] (W4a) and press [Go].
- (2) New tab will open for selected table (W4b), in which each protein domain/subunit is shown with domain SIRD-ID [ID], PDB code [PDB], chain ID [Chain], Domain number [DomainNo], first [Start] and last [End] amino acid, name of protein [Name], source organism [Organism], domain cluster ID [3Ddom], subunit cluster ID [3Dsub], and sequence cluster ID [1D], Keywords [Keyword1~5], etc...
- (3) This table is downloadable as tsv through [Download Table]

(W4a) View Table

2.3: View Table

Table: tbl0000

Go Reset

2.4: Delete Table

Table: tbl0000 ☐ all of mine

Go Reset

(W4b) Table

View table

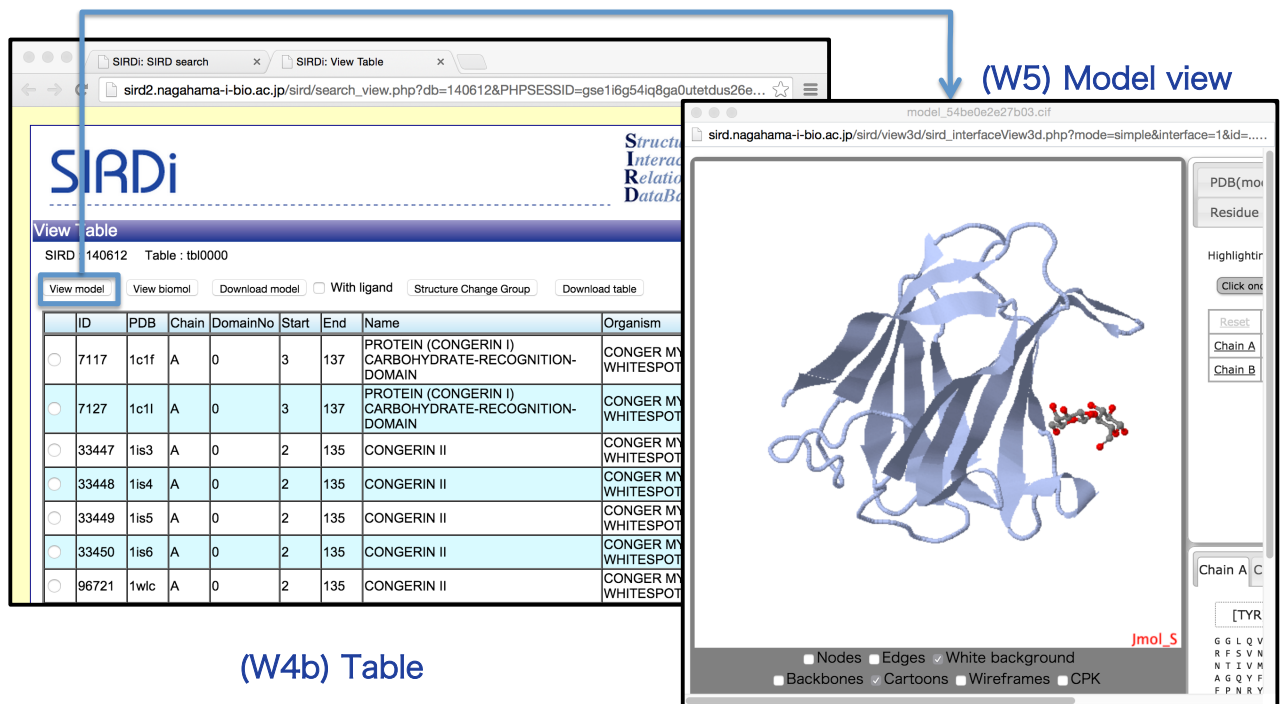
SIRD : 140612 Table : tbl0000

View model View biomol Download model ☐ With ligand Structure Change Group Download table

	ID	PDB	Chain	DomainNo	Start	End	Name	Organism
☐	7117	1c1f	A	0	3	137	PROTEIN (CONGERIN I) CARBOHYDRATE-RECOGNITION-DOMAIN	CONGER MYRI WHITESPOTTE
☐	7127	1c1l	A	0	3	137	PROTEIN (CONGERIN I) CARBOHYDRATE-RECOGNITION-DOMAIN	CONGER MYRI WHITESPOTTE
☐	33447	1is3	A	0	2	135	CONGERIN II	CONGER MYRI WHITESPOTTE
☐	33448	1is4	A	0	2	135	CONGERIN II	CONGER MYRI WHITESPOTTE
☐	33449	1is5	A	0	2	135	CONGERIN II	CONGER MYRI WHITESPOTTE
☐	33450	1is6	A	0	2	135	CONGERIN II	CONGER MYRI WHITESPOTTE
☐	96721	1wlc	A	0	2	135	CONGERIN II	CONGER MYRI WHITESPOTTE

How to view protein model

- (1) Select model by checking radio-button on top of each row on table (W4b)
- (2) Press [View Model] and model will be shown in new JSMOL window (W5)
- (3) If you also want to view interacting molecule check [With ligand] before pressing [View Model]



The image shows two windows from the SIRDi website. The left window, labeled (W4b) Table, displays a table of protein models. The right window, labeled (W5) Model view, shows a 3D protein structure in a JSMOL window.

(W4b) Table

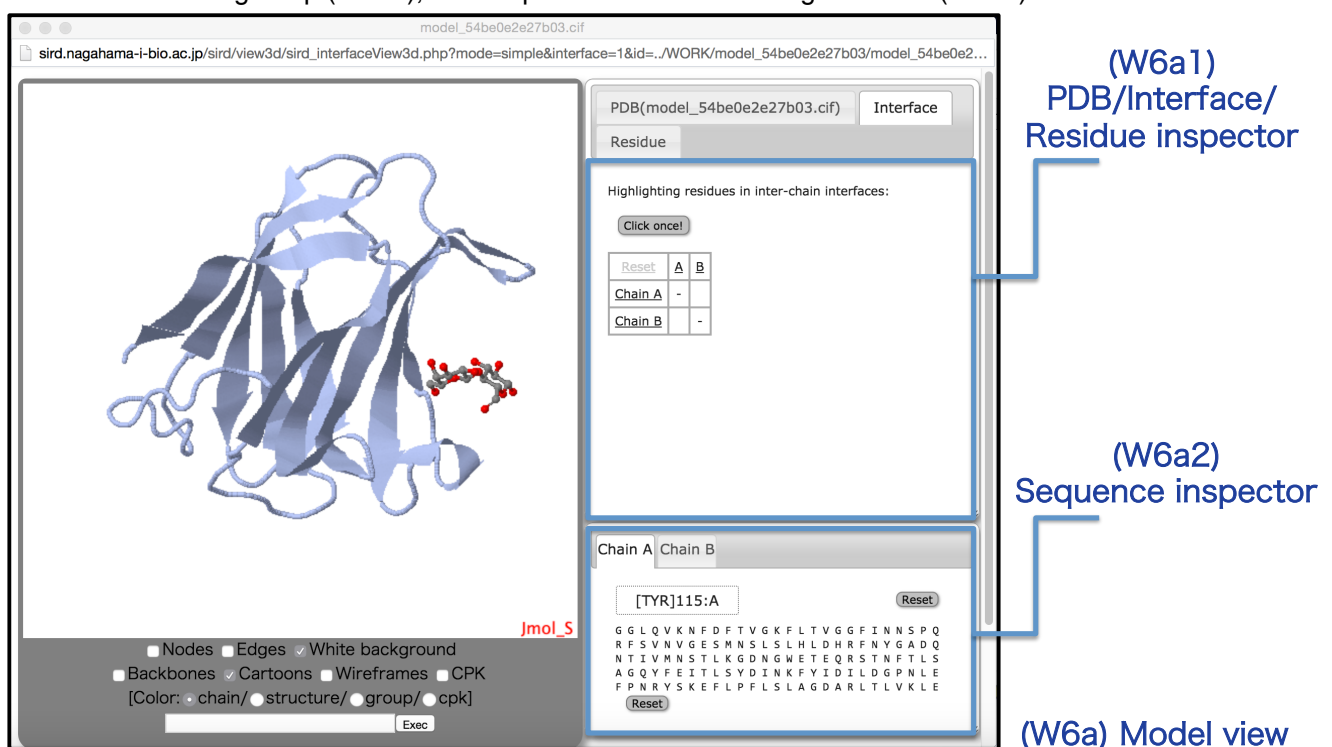
ID	PDB	Chain	DomainNo	Start	End	Name	Organism	
☐	7117	1c1f	A	0	3	137	PROTEIN (CONGERIN I) CARBOHYDRATE-RECOGNITION-DOMAIN	CONGER MY WHITESPOT
☐	7127	1c1l	A	0	3	137	PROTEIN (CONGERIN I) CARBOHYDRATE-RECOGNITION-DOMAIN	CONGER MY WHITESPOT
☐	33447	1is3	A	0	2	135	CONGERIN II	CONGER MY WHITESPOT
☐	33448	1is4	A	0	2	135	CONGERIN II	CONGER MY WHITESPOT
☐	33449	1is5	A	0	2	135	CONGERIN II	CONGER MY WHITESPOT
☐	33450	1is6	A	0	2	135	CONGERIN II	CONGER MY WHITESPOT
☐	96721	1wlc	A	0	2	135	CONGERIN II	CONGER MY WHITESPOT

(W5) Model view

The JSMOL window displays a 3D protein structure. The right sidebar shows the PDB(model) and Residue information. The bottom of the window has a toolbar with options like Nodes, Edges, White background, Backbones, Cartoons, Wireframes, and CPK.

JSMOL window

- (1) JSMOL window shows molecular graphic of selected complex (left window)
- (2) Header part of PDB file (PDB), Interface residues (Interface), neighboring residues (Residues) are shown in the right-top (W6a1), and sequences are shown in right-bottom (W6a2) windows.



The image shows the JSMOL window with a 3D protein structure on the left. The right side contains two panels: (W6a1) PDB/Interface/Residue inspector and (W6a2) Sequence inspector. The bottom of the window shows the model view options.

(W6a1) PDB/Interface/Residue inspector

PDB(model_54be0e2e27b03.cif) Interface

Residue

Highlighting residues in inter-chain interfaces:

Click once!

Reset

	A	B
Chain A	-	-
Chain B	-	-

(W6a2) Sequence inspector

Chain A Chain B

[TYR]115:A

Reset

```

GG LQ VKN FDF TVG KFL TV GGF INN SPQ
RF SV NV GES MNS LSL HLD HRF NY GADQ
NT IV MN STL KGD NGW ETE QR STN FTLS
AG QY FE ITL SYD INK FY IDI LDG PNL E
FP NR YS KE FL PFL SL AGD AR LTL VKLE
    
```

Reset

(W6a) Model view

Nodes Edges White background
Backbones Cartoons Wireframes CPK
[Color: chain/structure/group/cpk]

How to view biological molecular model

- (1) Select model by checking radio-button on top of each row on table (W4b)
- (2) Press [View Biomol] and model will be shown in new JSMOL (W6a) and SHOWGRAOH (W6b) windows

The screenshot shows three windows from the SIRD-i interface:

- (W4b) Table:** A table with columns ID, PDB, Chain, DomainNo, Start, and End. The first row is selected with a radio button.
- (W6a) Model view:** A 3D ribbon diagram of a protein structure in red and blue, with a Jmol.S logo.
- (W6b) Graph view:** A graph showing nodes (yellow circles) and edges (blue lines) representing the protein structure.

Arrows indicate the flow from the table to the model and graph views.

How to view derivative model (structure change pair)

- (1) Select model by checking left radio-button of each row on table (W4b)
- (2) Press [Structure Change Group] and new tab will open for the table of similar subunit/domains in different structure and/or interacting states
- (3) Select model by checking radio-button on top of each row on table (W7a)
- (4) Press [View model] and superposed models will be shown in new JSMOL window (W7b)

The screenshot shows two windows from the SIRD-i interface:

- (W7a) Table:** A table titled "Structure Change Group" with columns StID, StCode1, Status, ID, PDB, Chain, DomainNo, Start, End, and Name. The first row is selected with a radio button.
- (W7b) Model view:** A 3D ribbon diagram showing two superposed protein structures in green and blue, with a Jmol.S logo.

An arrow indicates the flow from the table to the model view.

How to search model with amino acid sequence

- (1) Click [2. SIRD search] at portal (W1)
- (2) Copy & paste your amino acid sequences in [Text (fasta)] box in [2_5: 1D Search] (W8a)
- (3) You may also upload sequence file through [File (fasta)]
- (4) Press [Go] and search will start

SIRD: SIRD search

2_5: 1D Search

By uploading fasta file or sequence

File(fasta)

Mail alert

or

Text (fasta)

Mail alert

or

By uploading mailed result file

File (result)

(W8a) 1D Search

- (5) After waiting for a moment (W8b), result will appear in new tab (W8c)
- (6) Each line in table shows similar subunit/domain with covered region in query sequence [=====], subunit/domain SIRD-ID [ID], coverage (%) [ORP], sequence identity (%) [IDN], PDB code/Chain/Domain No [PDB/C/N], domain cluster ID [3Ddom], subunit cluster ID [3Dsub], and sequence cluster ID [1D]
- (7) Check right radio-button of each low on table, fill top-right box with new table name and press [Make] will make a table with selected subunit/domains

SIRD: 130927 Job ID : 1d_52c125c5d67cc

1D Search

Table

	ID	ORP	IDN	PDB/C/N	3Ddom	3Dsub	1D	
=====	00446027	100	94	4dqyF-01	-00001	008901	013781	☐
=====	00446028	100	94	4dqyF001	009831	008901	013781	☐
=====	00446029	100	94	4dqyF002	000909	008901	013781	☐
=====	00446022	100	94	4dqyC-01	-00001	008901	013781	☐
=====	00446023	100	94	4dqyC001	009831	008901	013781	☐
=====	00446024	100	94	4dqyC002	000909	008901	013781	☐
=====	00217875	100	100	2rcwA-01	-00001	001122	000897	☐
=====	00217876	100	100	2rcwA001	003806	001122	000897	☐
=====	00217877	100	100	2rcwA002	002065	001122	000897	☐
=====	00217878	100	100	2rcwA003	000909	001122	000897	☐
=====	00120076	100	100	1wokD-01	-00001	001122	000897	☐
=====	00120077	100	100	1wokD001	003806	001122	000897	☐
=====	00120078	100	100	1wokD002	002065	001122	000897	☐
=====	00120079	100	100	1wokD003	000909	001122	000897	☐
=====	00120072	100	100	1wokC-01	-00001	001122	000897	☐
=====	00120073	100	100	1wokC001	003806	001122	000897	☐

(W8b) Waiting

(W8c) Result table

How to search for ligand molecules

- (1) Press [**LIGDIC**] in [2_1: Select - Ligand] (**W3a**)
- (2) A new window will open for Ligand Dictionary (**W9a**)
- (3) Fill boxes in [LIGand DICTIONary] with your search conditions as many as you want (e.g. ligand ID for [ID], ligand cluster ID for [Group ID], PDB 3L code for [Code], name of ligand molecule for [Name], chemical formula of ligand for [Formula])

(W9a) Ligand selection window

(W3a) Selection window

- (4) Press [**Search**] and result will appear under this window (**W9b**)
- (5) Model of ligand will be shown in new JSMOL window by check right radio-button of each row on table and press [**View model**] (**W9c**)
- (6) Press [**Select**] will put selected PDB 3L codes into search box on [2_1: Select – Ligand] (**W3a**)

(W9c) Ligand model view

(W3a) Selection window

(W9b) Ligand table

ID	GroupID	Code	Name	Formula	
7	10	DA	2'-DEOXYADENOSINE-5'-MONOPHOSPHATE	C10 N5 O6 P1	☒
21	685	ALA	ADENOSINE-5'-MONOPHOSPHATE	C3 N1 O2	☐
54	176	UPA	URIDYL-2'-5'-PHOSPHO-ADENOSINE	C19 N7 O12 P1	☐
62	10	AMP	ADENOSINE MONOPHOSPHATE	C10 N5 O7 P1	☐
71	21	ADP	ADENOSINE-5'-DIPHOSPHATE	C10 N5 O10 P2	☐
90	10	A	ADENOSINE-5'-MONOPHOSPHATE	C10 N5 O7 P1	☐
96	12	A2M	2'-O-METHYLADENOSINE 5'-(DIHYDROGEN PHOSPHATE)	C11 N5 O6 P1	☐

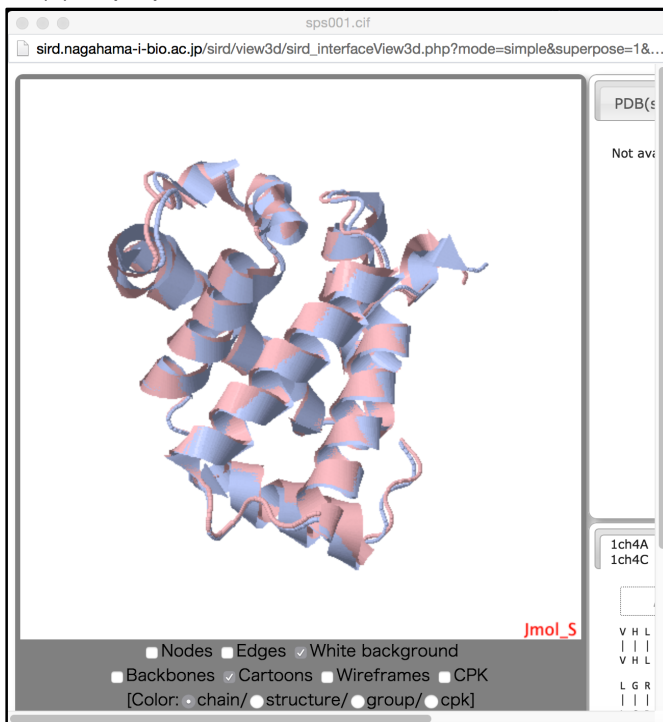
How to superpose protein structures

- (1) Press [3. SIRD modeling] at portal (W1) and go to [3_1: Superpose subunit] (W10a)
- (2) Upload PDB file or enter PDB code [Code1] and chain [Chain] for subunit 1
- (3) Upload PDB file or enter PDB code [Code2] and chain [Chain] for subunit 2
- (4) Thresholds for superposition might be changed for [Coverage >] (% for superposed region in total) and [RMSD <] for maximum r.m.s.d (Å)
- (5) Check radio-button [View model] to view model, and check [With ligand] to view interacting molecules also
- (6) Press [Go] will start calculation

(W10a)
Superpose subunit

(7) Result will appear as structural sequence alignment in new tab (W10b)

(8) Superposed model will be shown in new JSMOL window if [View model] was checked (W10c)



(W10c) Superposed model

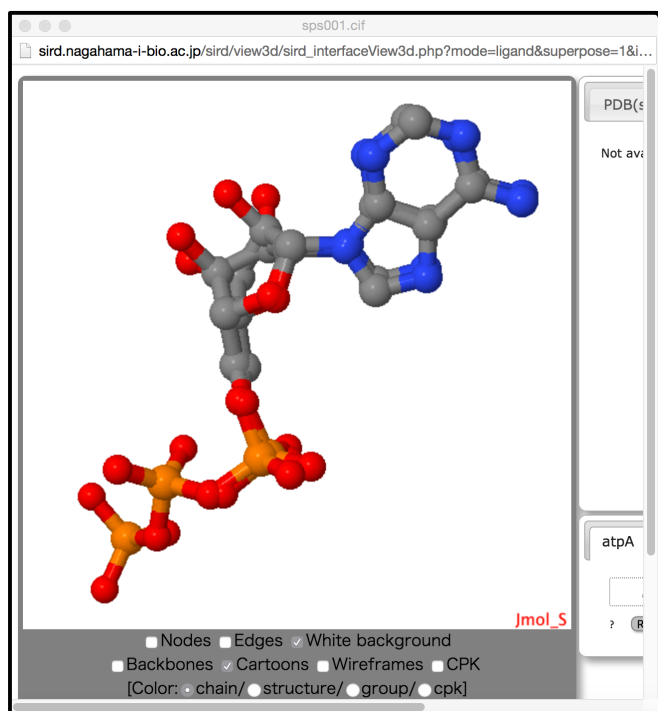
(W10b) Superpose result

How to superpose ligand (small molecule) structures

- (1) Click [[3. SIRD modeling](#)] at portal ([W1](#)) and go to [[3_5: Superpose ligand](#)] ([W11a](#))
- (2) Upload PDB file of ligand molecule or enter PDB 3L code [Code1] for ligand1
- (3) Upload PDB file of ligand molecule or enter PDB 3L code [Code2] for ligand2
- (4) Thresholds for graph matching might be changed for [M(A,B)/M(A)] (fraction of matched atoms/bonds in ligand1) and/or [M(A,B)/M(B)] (fraction of matched atoms/bonds in ligand2)
- (5) Check radio-button [[View model](#)] to view model
- (6) Press [[Go](#)] will start calculation

(W11a)
Superpose ligand

- (7) Result will appear as atom alignment in new tab ([W11b](#))
- (8) Superposed model will be shown in new JSMOL window if [[View model](#)] was checked ([W11c](#))



(W11c) Superposed model

NAM	NoA	MSC	MAX	RMSD	NoS	ALIGNMENT
ATP	31	64	64	0.000	31	PG 01G 02G 03G PB 01B 02B 03B PA 01A 02A 03A
AMP	23	42	48	0.175	21	----- P 02P. 03P. 01P

(W11b) Graphmatch result

Copyright (C) 2015 SIRD committee
This work was supported by BIRD and PDIS