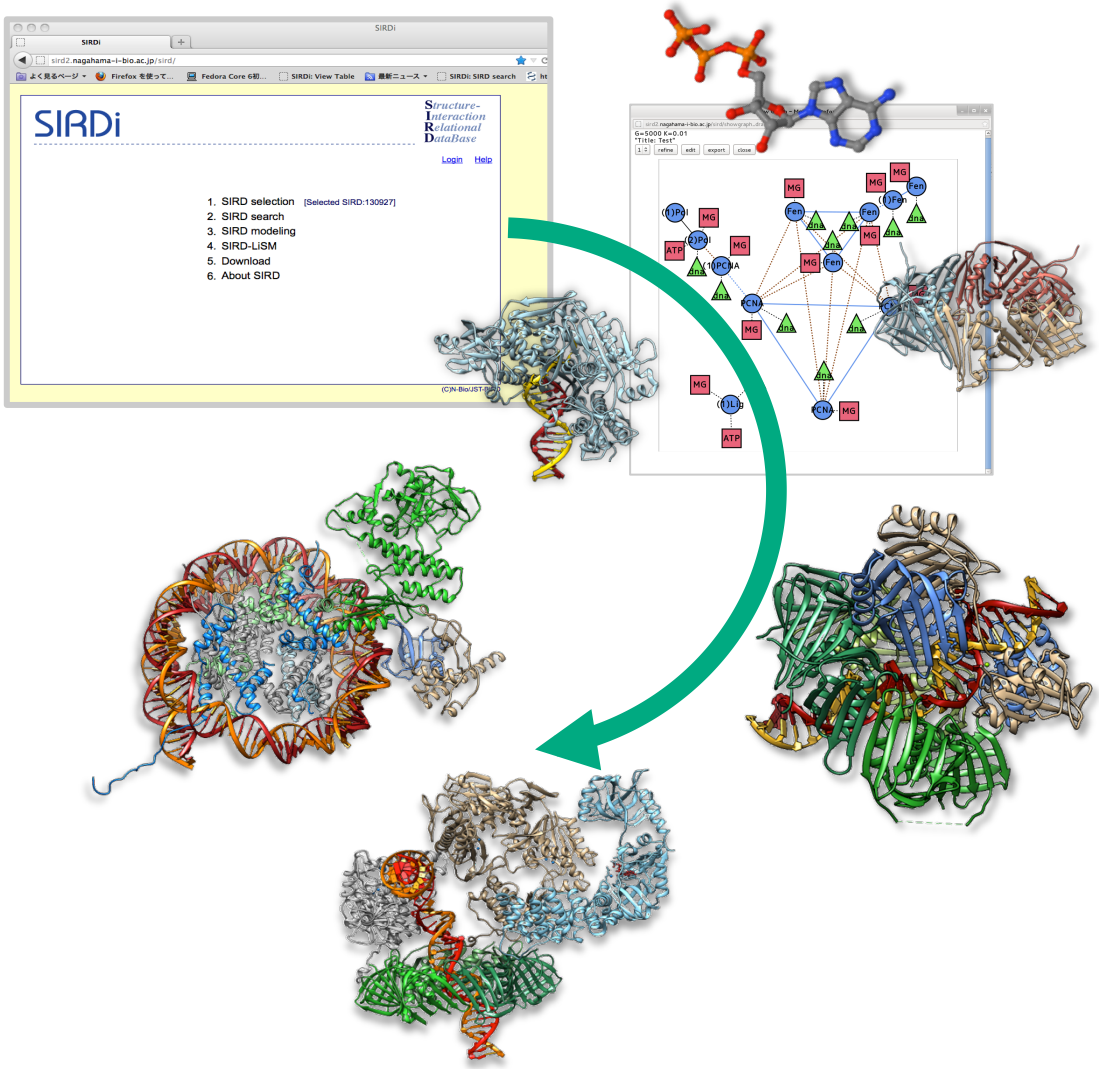
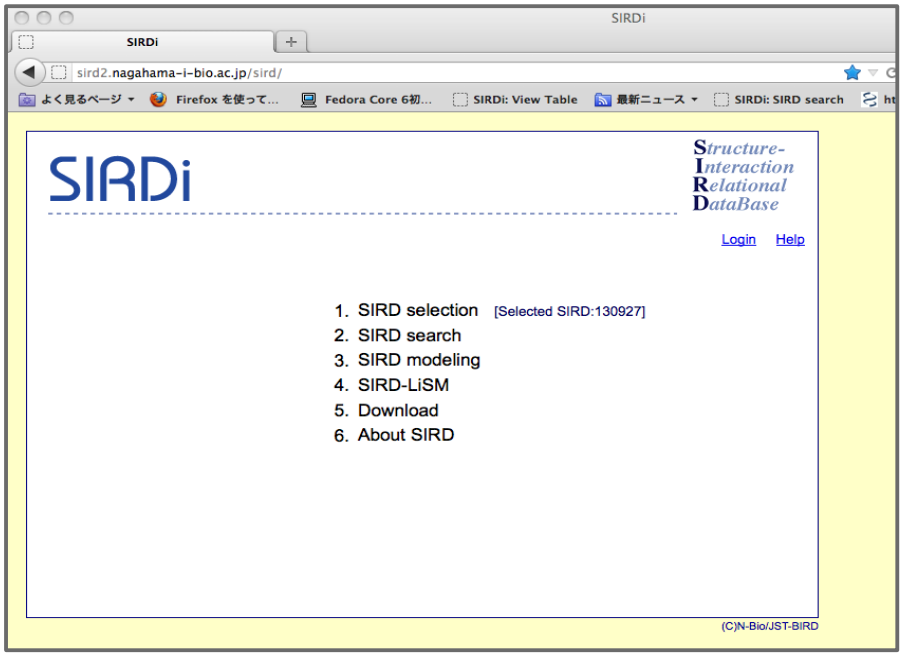
Easy manual for SIRD interface



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



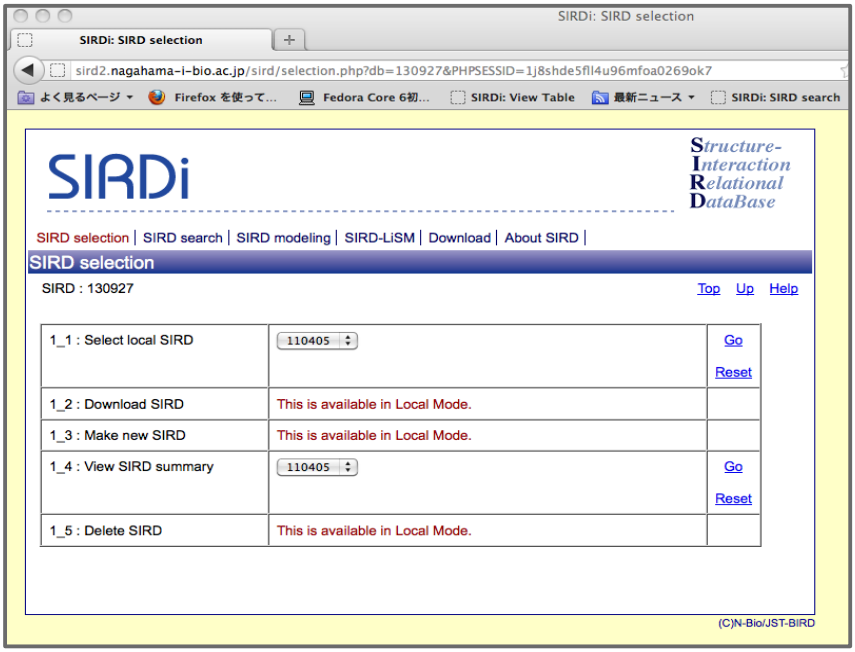
(W1) SIRDi portal

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)

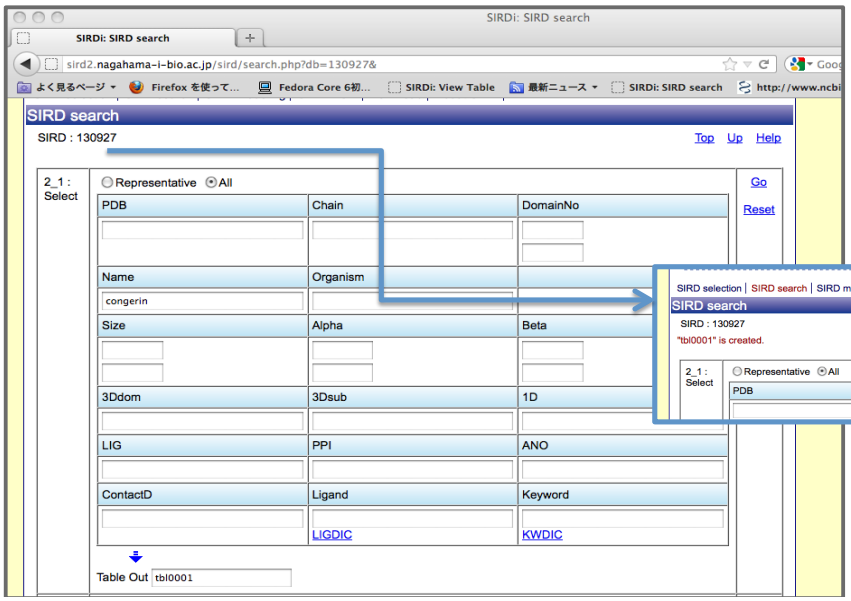
(3) Summary for each database can be viewed through [1_4: View SIRD summary]



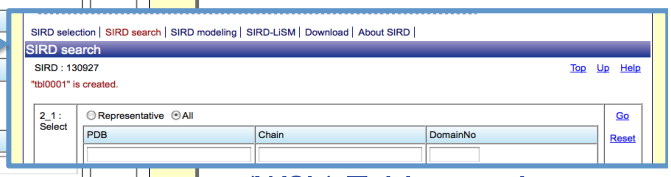
(W2) DB selection

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.



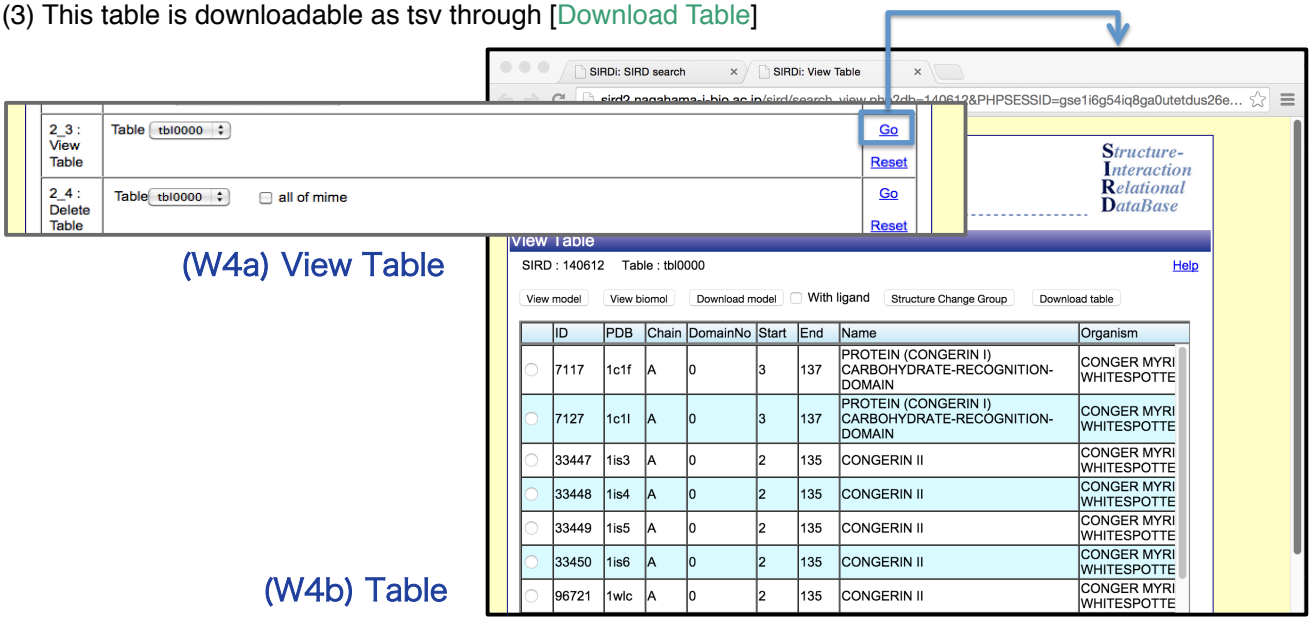
(W3a) Selection window



(W3b) Table creation

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

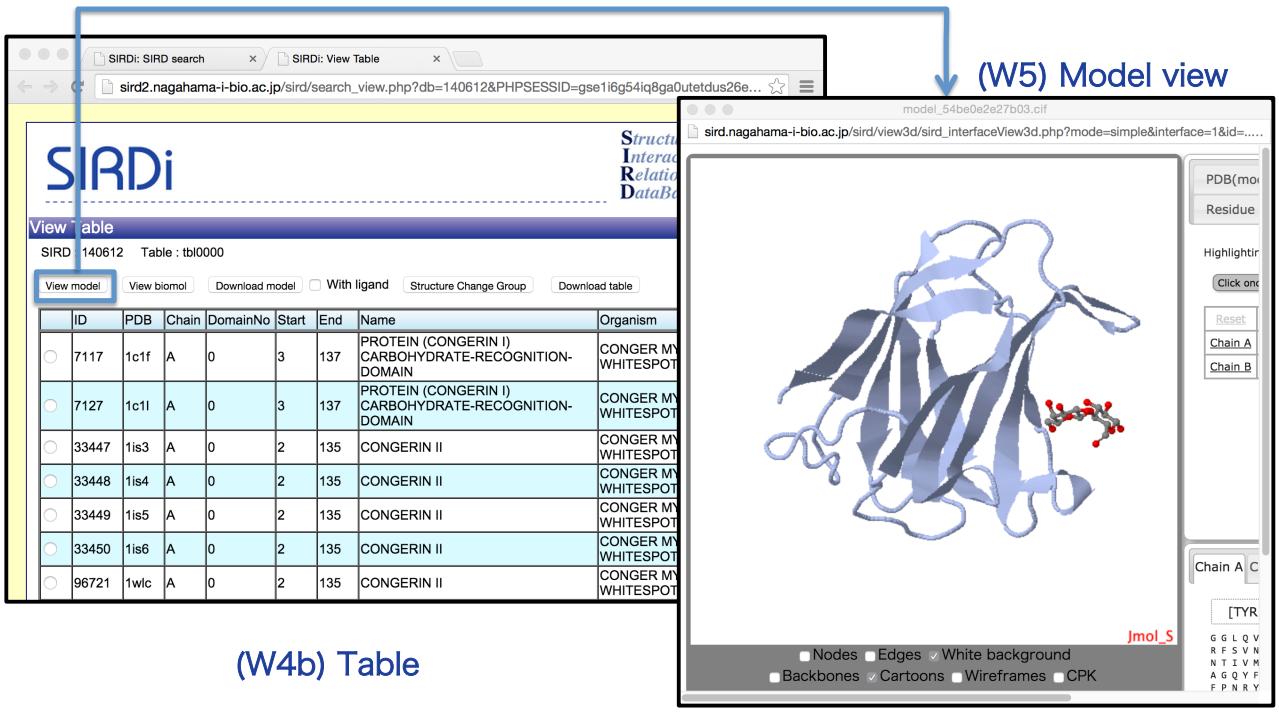
(W4b) Table

How to view protein model

(1) Select model by checking radio-button on top of each low on table (W4b)

(2) Press [View Model] and model will be shown in new JSMOL window (W5)

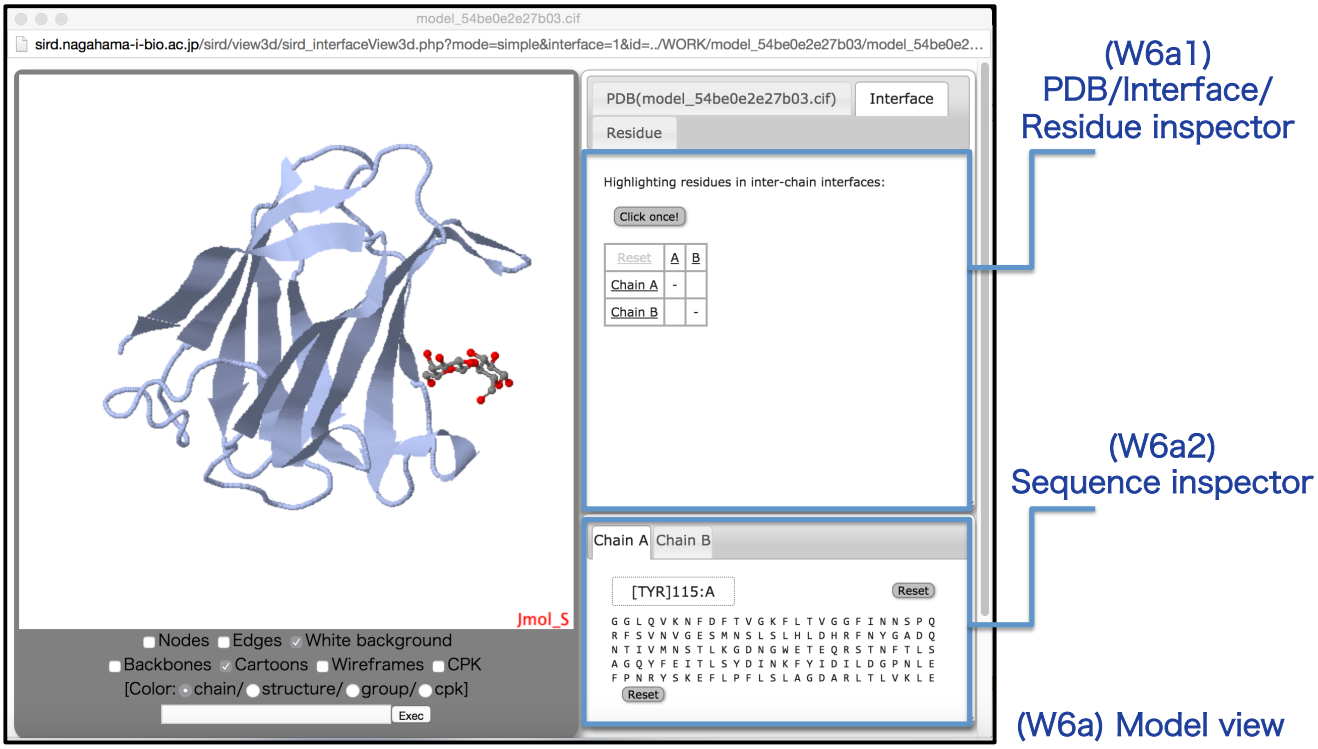
(3) If you also want to view interacting molecule check [With ligand] before pressing [View Model]



JSMOL window

(1) JSMOL window shows molecular graphic of selected complex (left window)

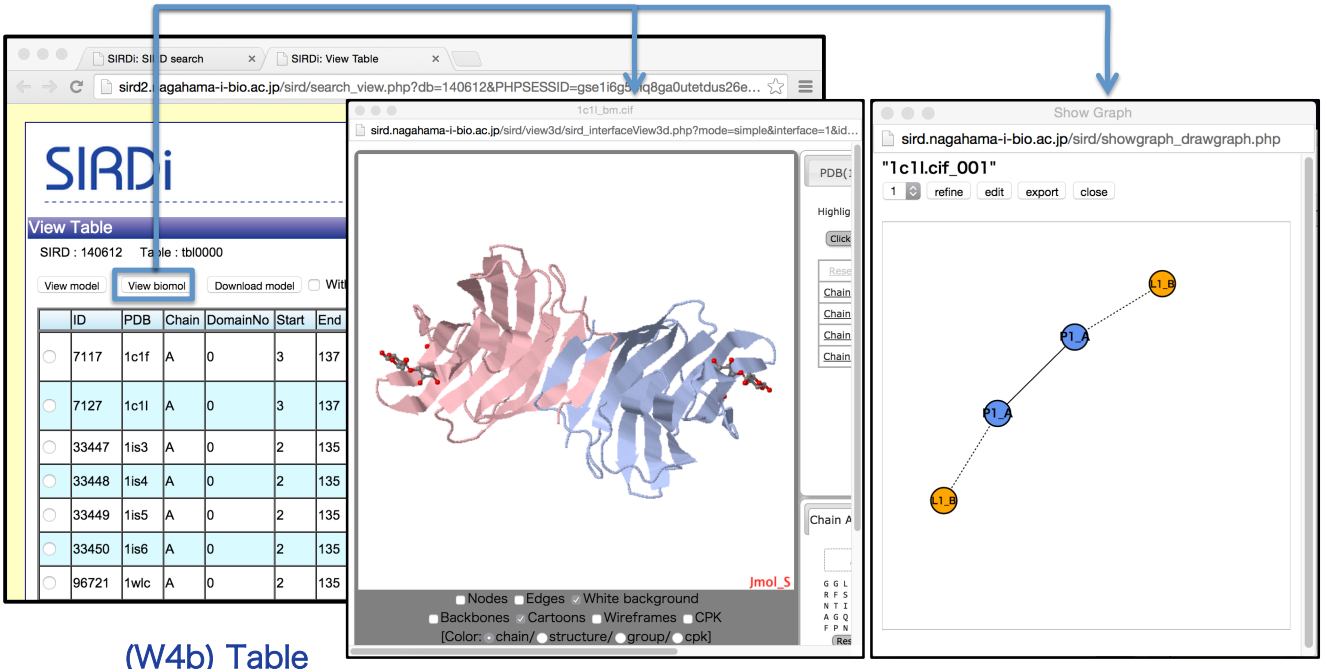
(2) Header part of PDB file (PDB), Interface residues (Interface), neighboring residues (Residues) are shown in the right-top (W6a1), and sequences are shown in right-bottom (W6a2)windows.



How to view biological molecular model

(1) Select model by checking radio-button on top of each low on table (W4b)

(2) Press [View Biomol] and model will be shown in new JSMOL (W6a) and SHOWGRAOH (W6b) windows



(W4b) Table

(W6a) Model view

(W6b) Graph view

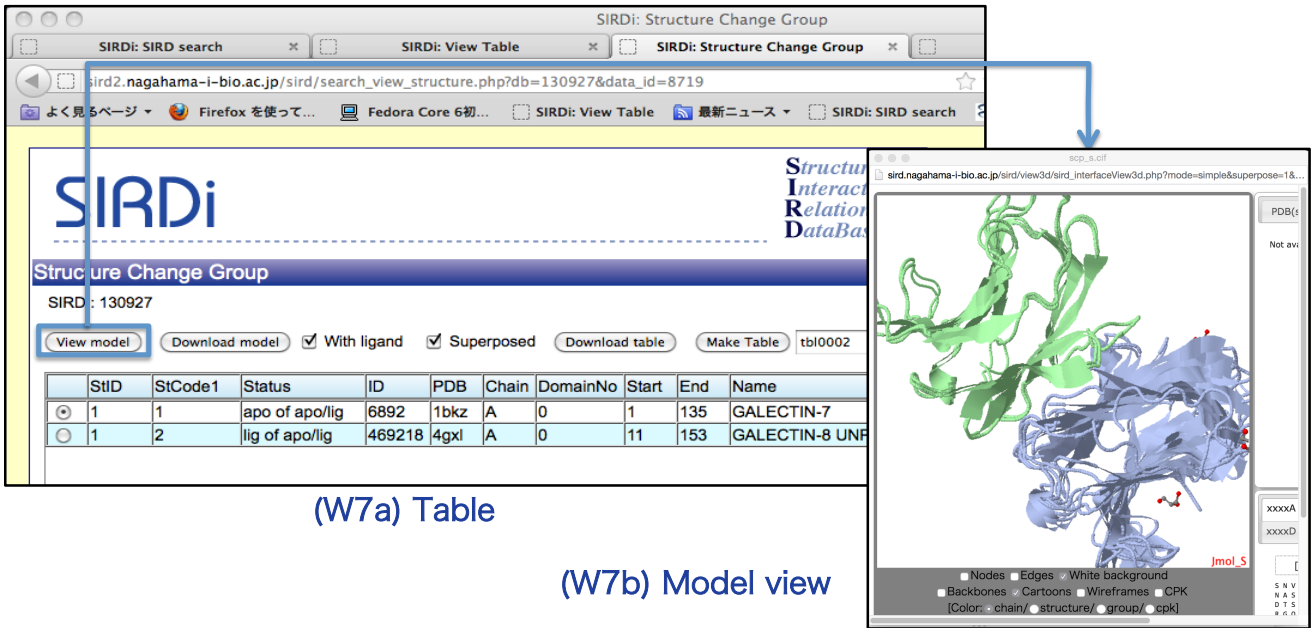
How to view derivative model (structure change pair)

(1) Select model by checking left radio-button of each low 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 low on table (W7a)

(4) Press [View model] and superposed models will be shown in new JSMOL window (W7b)



(W7a) Table

(W7b) Model view

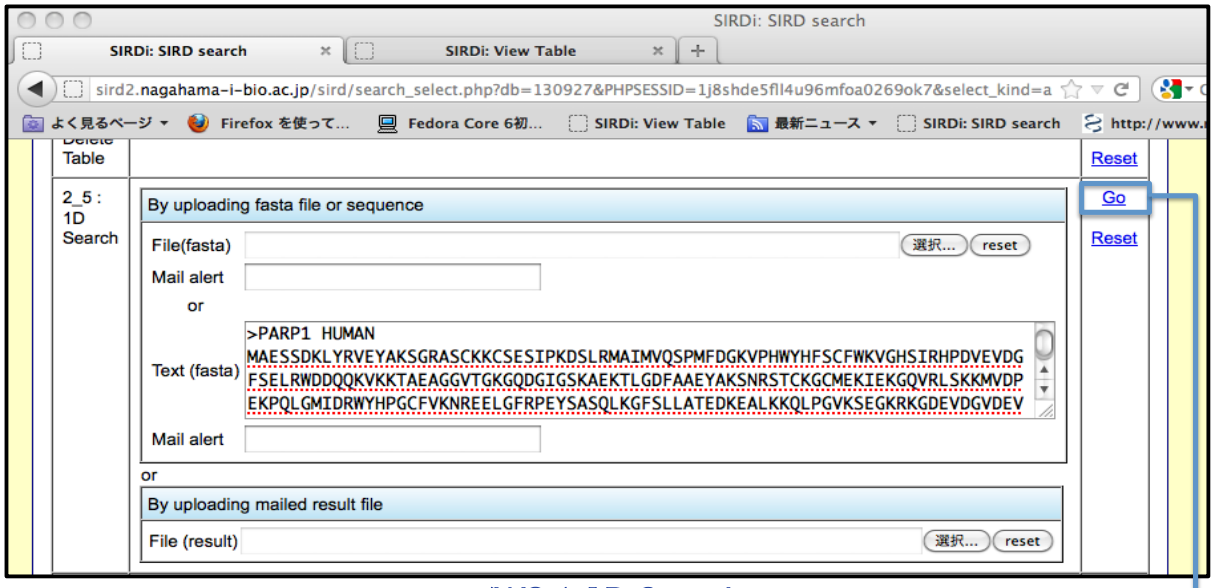
How to search model with amino acid sequence

(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 (fatsa)]

(4) Press [Go] and search will start

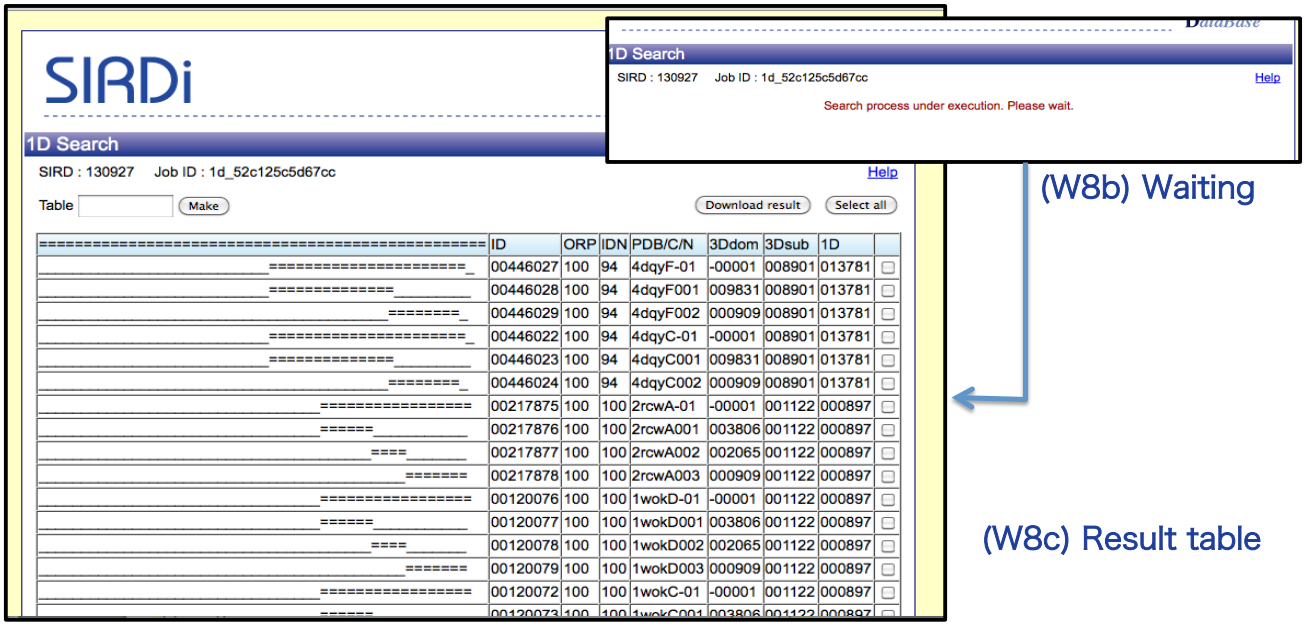


(W8a) 1D Search

(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



(W8b) Waiting

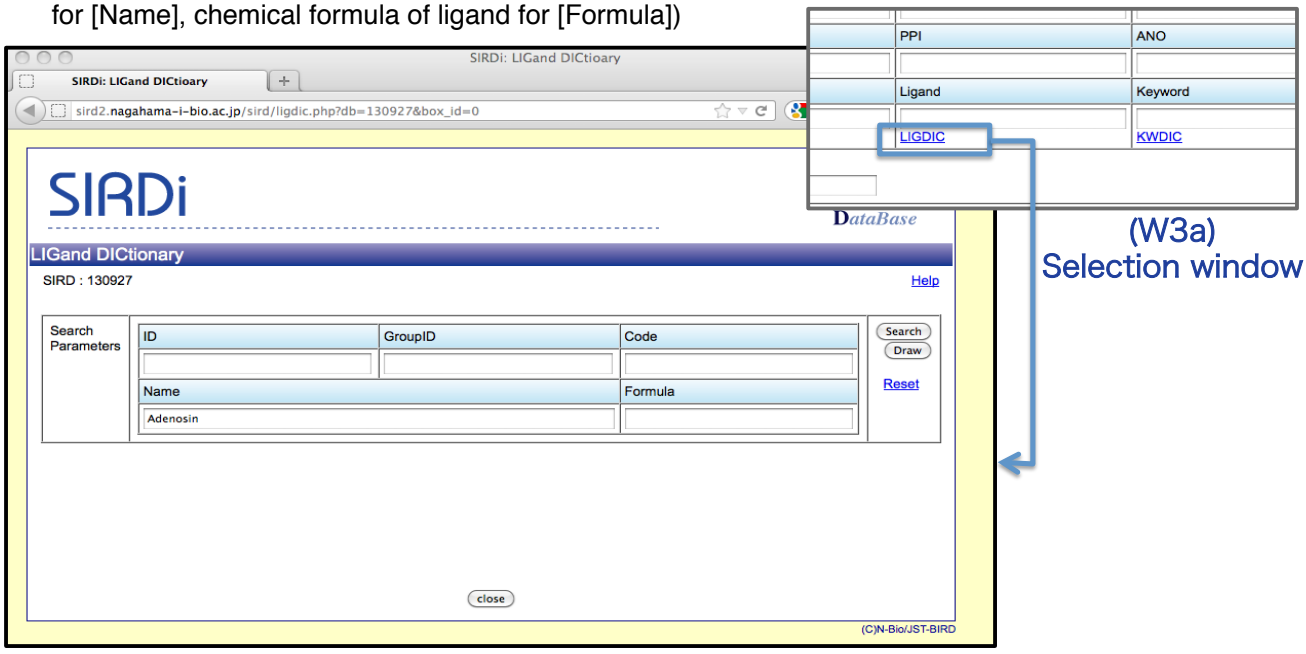
(W8c) Result table

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

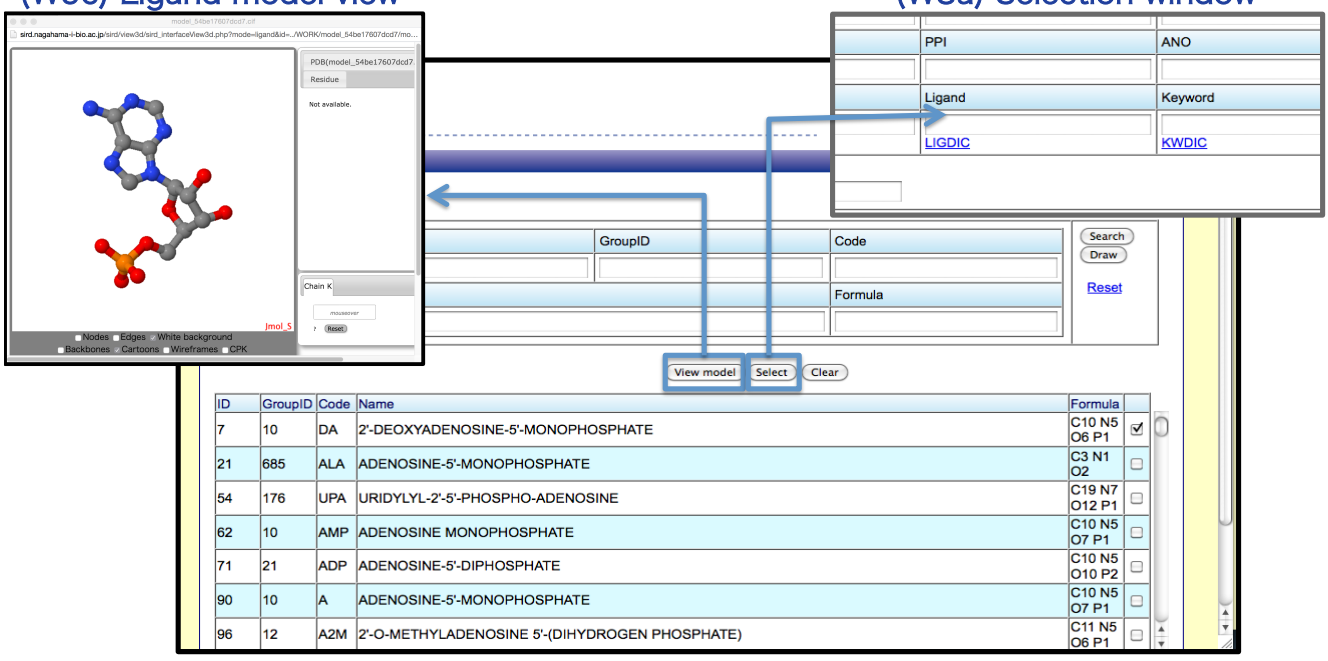
(4) Press [Search] and result will appear under this window (W9b)

(5) Model of ligand will be shown in new JSMOL window by check right radio-button of each low 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

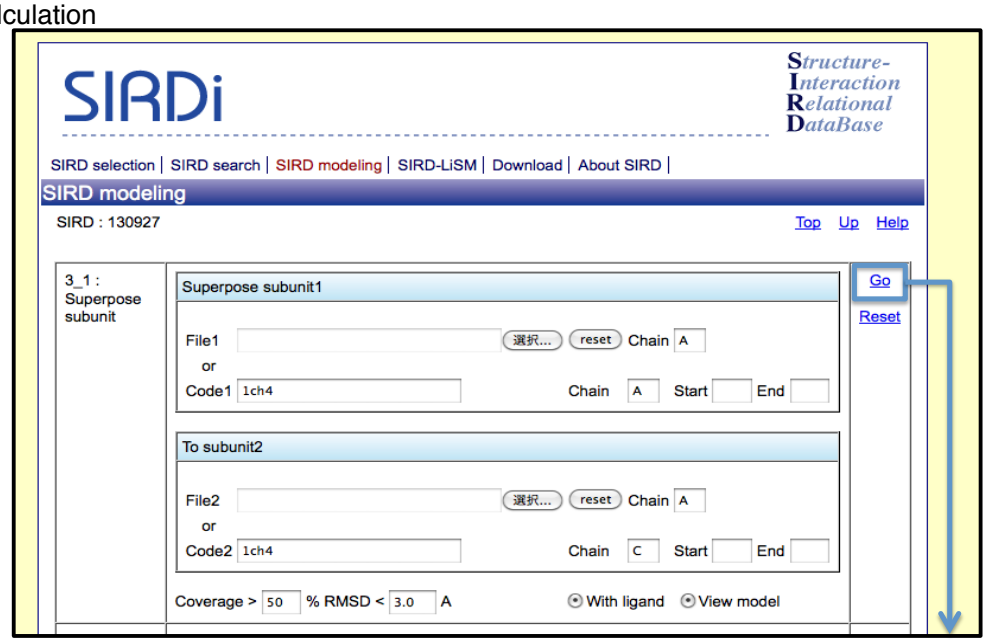


(W9b) Ligand table

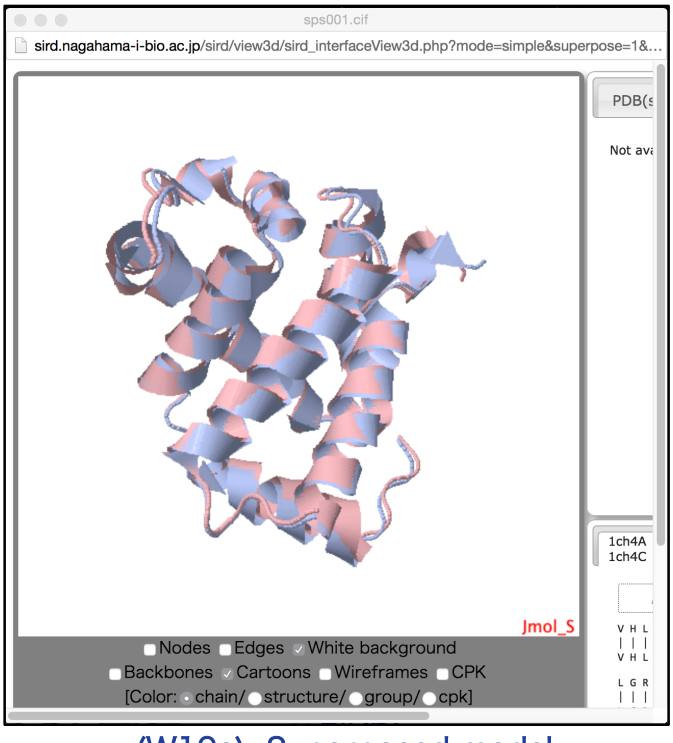
How to superpose protein structures

(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 (A)
(5) Check radio-button [View model] to view model, and check [With ligand] to view interacting molecules also
(6) Press [Go] will start calculation

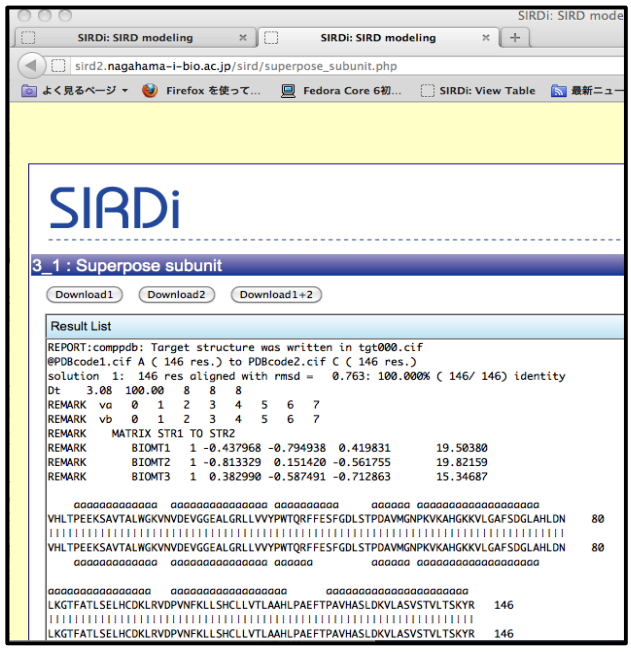
(W10a)
Superpose subunit



(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 logand] (W11a)

(2) Upload PDB file of ligand molecule or enter PDB 3L code [Code1] for ligand1

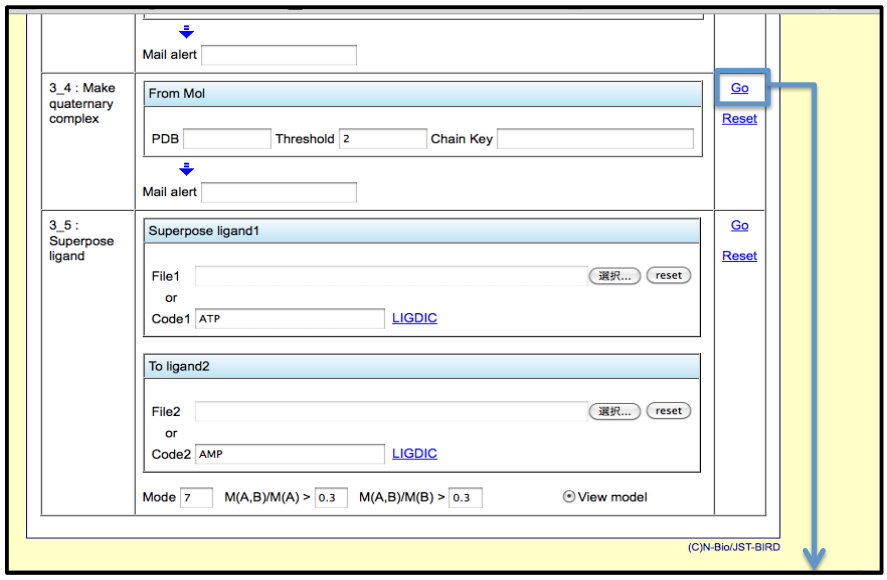
(3) Upload PDB file of ligand molecule or enter PDB 3L code [Code2] for ligand2

(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

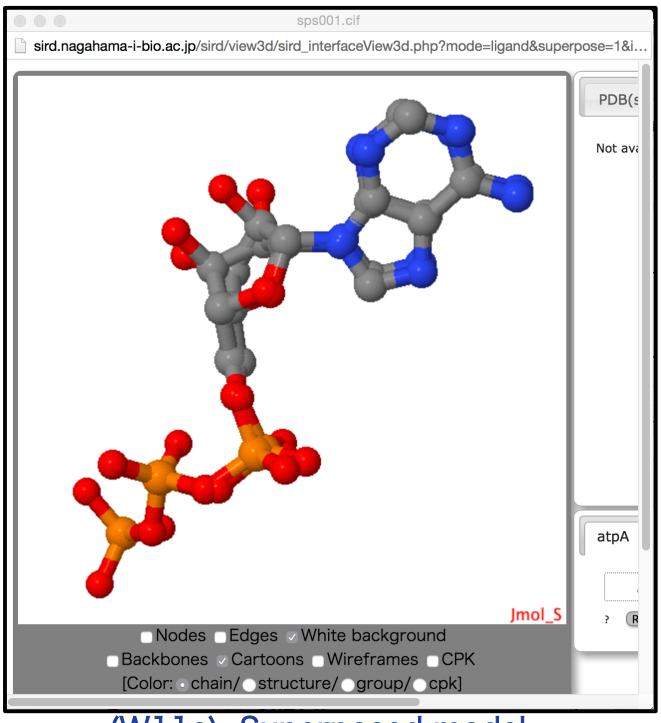
(6) Press [Go] will start calculation

(W11a)
Superpose ligand

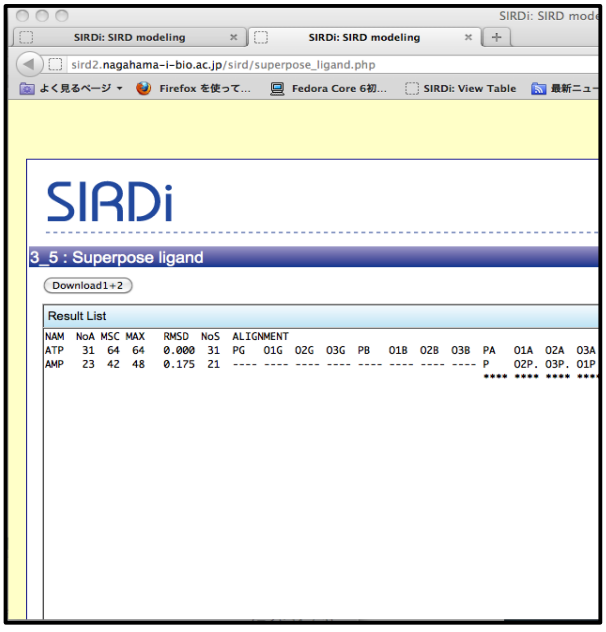


(7) Result will appear as atom alignment in new tab (W11b)

(8) Superposed model will be shown in new JSMOL window if [View model] was checked (W11c)



(W11c) Superposed model



(W11b) Graphmatch result

This work was supported by BIRD and PDIS