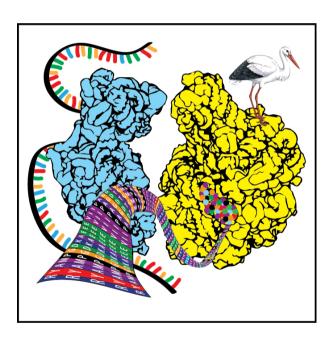
User manual IBiSS

UBiSS can be used from any web browser. There is no need for additional installation. If your browser does not have the Java plugin installed, it will prompt you to install it. Javascript must be enabled on your browser. For your visual comfort, a 17 inch screen or more is recommended. (however the site is usable on smaller screens). Firefox and Chrome browsers are recommended, especially for the management of Java applets.



Beinsteiner Brice, Klaholz Bruno

The Institute of Genetics and of Molecular and Cellular Biology (IGBMC),

University of Strasbourg, FRANCE

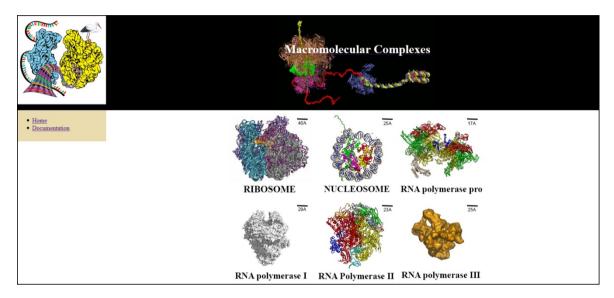
Summary

I) The choice of the complex
II) The different tools
1) All proteins for one species
A) The choice of the species
B) Le result
2) All species for one protein
A) The choice of protein
B) The result
a) The table4
b) Alignment Tab4
c) Sequence Tab5
d) 3D tab5
e) Taxonomy Tab7
f)References Tab
3) Compare species
A) The choice of species.
B) Result8
4) Taxonomy complex
5) Coevolution9
A) Taxonomic tree tab9
B) Alignment tab
Guide to use the consol Jmol
For more information

I) The choice of the complex

On the home page, select the complex as of interest.

There are 9 complexes presented as thumbnails. A 10th thumbnail called "SINGLE PROTEIN" is present. It includes initiation factor monomer.



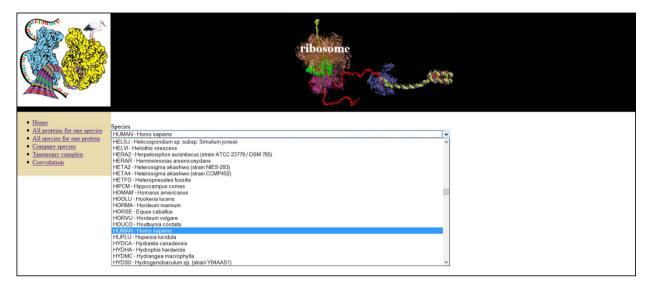
II) The different tools

- Home
- All proteins for one species
- All species for one protein
- Compare species
- Taxonomy complex
- Coevolution

1) All proteins for one species.

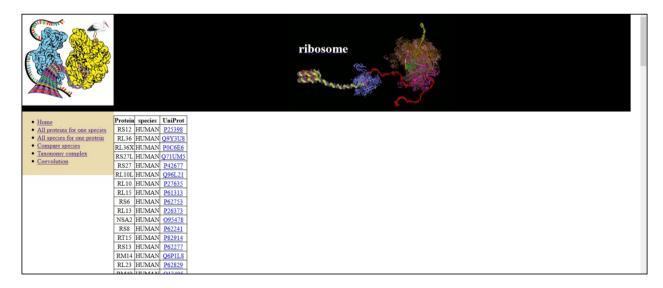
A) The choice of the species.

There is a list of species available for the selected complex. This means that no species proposed will give a null result. Simply choose a species and then submit.



B) Le result

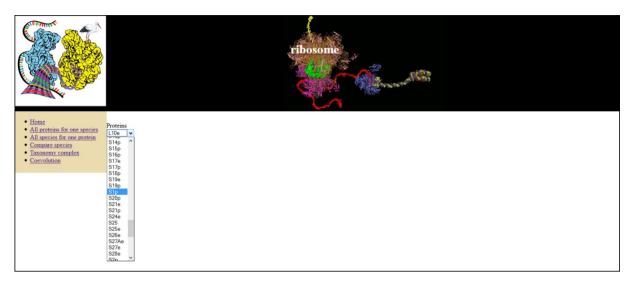
The result is in the form of a table that lists all the available protein for the complex studied and the selected species. The information is the name of the protein, the species and the link to Uniprot. This functionality is used to make a rapid assessment of the performance of the species in the database for the selected complex.



2) All species for one protein.

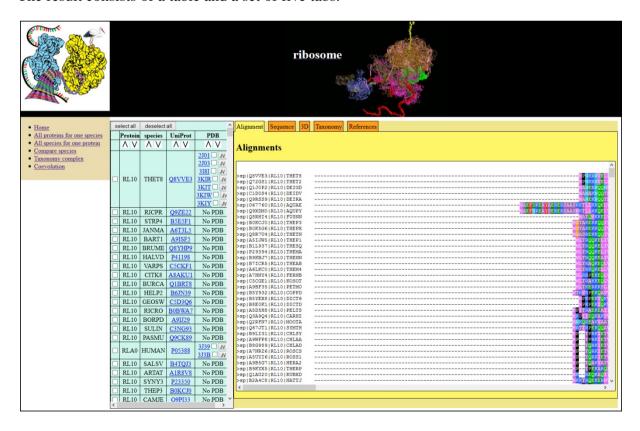
A) The choice of protein

There is a list of component protein complex (and variant). Once selected simply submit.



B) The result

The result consists of a table and a set of five tabs.



a) The table

It consists of five columns, 3 are informative and 2 are functional.

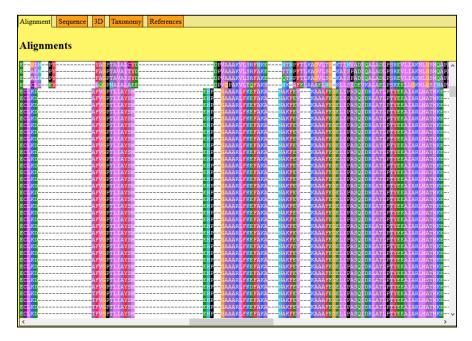
The Protein column shows the name of the protein, the Species column shows the name of the species and the UniProt column gives the link to the sequence database UniProt.

The first unnamed column is composed of a checkbox by protein. Just click on it to select it, the effect is visible on the tabs and Sequence References and be seen later in the parties Sequence Tab and References Tab. To use the last PDB column must 3D page is visible so that the applet is initialized. It indicates the presence or absence of PDB file, if a PDB file is available, three functional elements are assigned, the PDB number is clickable, a check box and a button JV. Their usefulness will be seen in the 3D tab part.

Protein	species	UniProt	PDB
Λ	^ V	Λ∨	Λ٧
RL10	THET8	Q8VVE3	2J01 JV 2J03 JV 3I8I JV 3KIR JV 3KIT JV 3KIW JV 3KIY JV
RL10	RICPR	Q9ZE22	No PDB
RL10	STRP4	<u>B5E5F1</u>	No PDB
RL10	JANMA	<u>A6T3L5</u>	No PDB
RL10	BART1	A9ISF5	No PDB
RL10	BRUME	Q8YHP9	No PDB
RL10	HALVD	P41198	No PDB
RI.10	VARPS	C5CKF1	No PDB

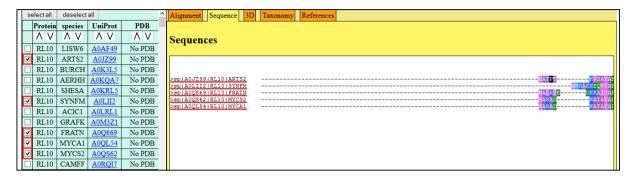
b) Alignment Tab

Alignment tab is the default tab. It has an overall alignment of the whole protein for this protein family. The alignment is pre-calculated with clustal W. The header of each sequence alignment indicates the PDB identifier, the name of the protein and the species. The alignment is diplayed in a fixed sized and scrollable windows.



c) Sequence Tab

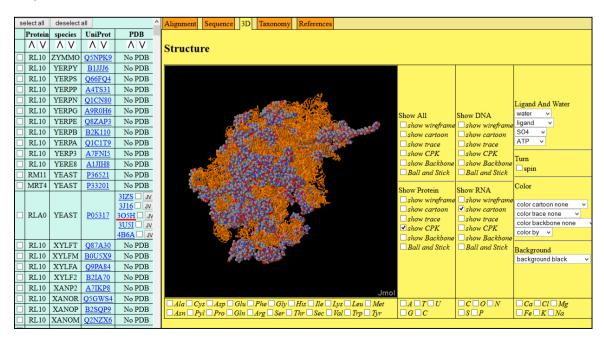
By default, the Sequence tab is empty. This is similar to the overall alignment part. But the overall alignment is not practical if you want to compare a limited number of sequence that are not side by side in alignment. If we compare these specific sequences, one needs only to to identify them in the table of results and check the check box in the first column. The selected sequences are added in the order of selection.



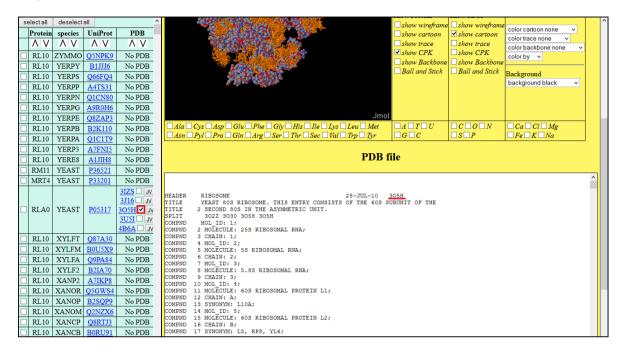
d) 3D tab

Important Note: Depending on the browser and browser version, it may be that when you change the tab, the Java applet is disabled then recharges when the returns are on this tab. In some cases the tab change does not cause stopping applet. This property is specific to the browser as well as its version and can change from one version to another for the same browser.

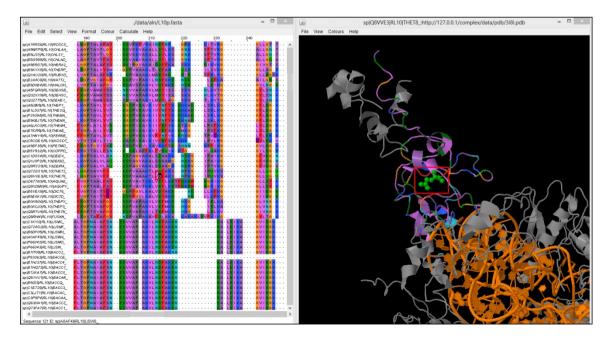
To properly use this tab it is required that the java plugin is installed in your browser. Once the tab is loaded, the java applet is automatically or request your permission loaded according to the permissions of the browser. This tab is divided into two parts. The first part is a Jmol applet with a user interface in JavaScript. The second part is a text box named PDB File. This is where the PDB column is useful. Just click on the PDB identifier for the structure load in the Jmol applet, so it is possible to see very quickly all structures present in this protein family.



The checkbox next to the PDB identifier allows you to view the contents of the PDB file as a text in the PDB file part. This is useful for even the composition of the structure if it is a complex and comments in the file.

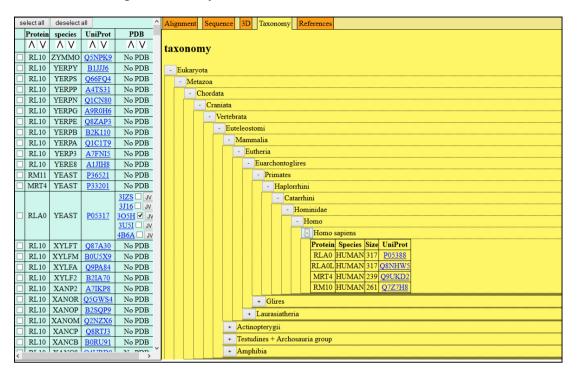


The last JV button, creates an applet button between the two parts that call Start Jalview. Simply click above to create two new window, Jalview window that contains the sequence alignment, as well as associated Jmol window which contains the selected structure that is directly aligned with the corresponding sequence of the overall alignment. Thus there are two new window linked interactively which can be full screen on two different screens if the machine you are using has two or more screens. It is convenient to generate multiple pairs of Jalview - Jmol windows simultaneously. The "JV" button allows loading of the applet start button to access the Jmol and Jalview window.



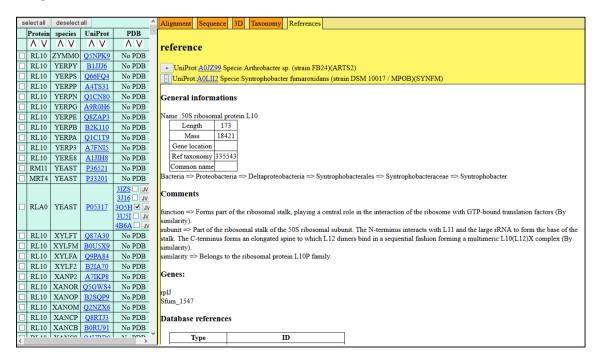
e) Taxonomy Tab

This tab allows you to navigate through a taxonomic tree that contains only the species present in the studied protein family.



f)References Tab

References tab meanwhile can View all information known about a sequence and all links to other database about the same protein. To see the details of a protein, one must select the check box by the first column of the table. This is the same checkbox that adds a sequence to the Sequence tab and adds additional information References tab.

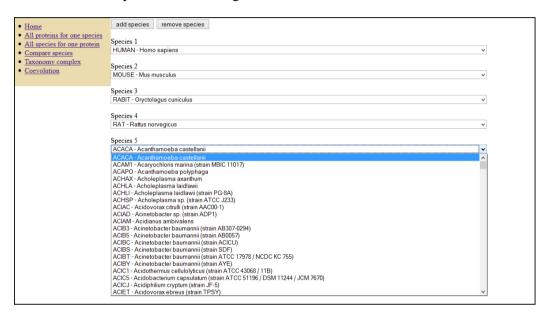


3) Compare species

A) The choice of species.

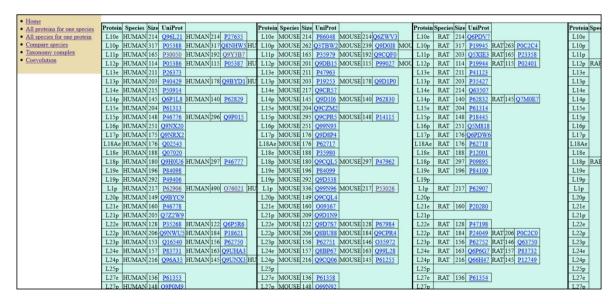
There is a list of species available for the selected complex. This means no species proposed will give a zero result. Simply choose the species and then submit it. There is no limit to the number of species to compare.

Warning, the absence of a protein in a species does not necessarily mean that the protein is not present in vivo. Only that it is missing from the database.



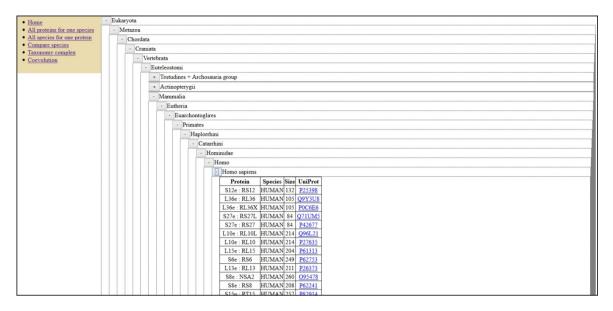
B) Result

the result is in the form of tables which include all the proteins of the complex. A blank line means that there is no protein present in the database.



4) Taxonomy complex

This page allows you to browse through a taxonomic tree that contains only the species present in the complex studied.

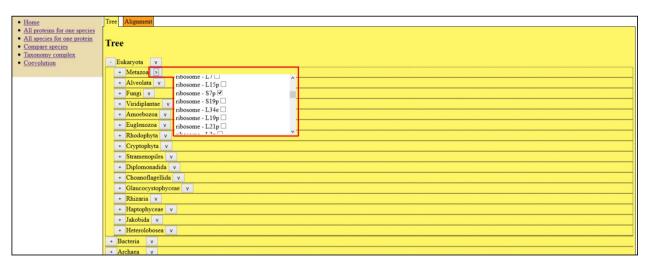


5) Coevolution

The Coevolution page is composed of two tabs.

A) Taxonomic tree tab

With this tab we have access to all species of database in a taxonomic tree. It is possible for each taxon to access a list of proteins for which at least one member of a taxon sequence. Beside each protein there is a checkbox, simply select proteins of interest for the taxon of your choice.



B) Alignment tab

In the Alignment tab, displays alignment division taxon specific sequences and protein selected. There is no limit to the number of different alignments that would have displayed. Each alignment corresponds to a taxon and a protein. The sequence alignment is precalculated.



Guide to use the consol Jmol

Load structure directly from the server:

load ./data/pdb/1K73.pdb

Select:

Select all:

select all

Select elements:

select carbon

Select chains:

select *:F

Select a type of amino acid:

select [HIS]

Select a type of amino acid of chain:

select [HIS]:F

Select a macromolecule:

select protein

Select a specific amino acid:

select 95:F

Change the display:

cpk on / cpk off

change the size of balls:

cpk 0.5

wireframe on

cartoon on

trace on

backbone on

motion:

move [x-rotation] [y-rotation] [z-rotation] [zoom-factor] [x-translation] [y-translation] [z-translation] [slab-cutoff] [seconds-total] [move-frames-per-second] {default: 30} [maximum-acceleration] {default: 5}

example:

move 10 180 90 0 0 0 0 5

change color:

color red

For more information

Jmol tutorial:

- http://www.chem.uwec.edu/JmolTut/index.html

Jalview tutorial:

- http://www.jalview.org/tutorial/TheJalviewTutorial_screen.pdf

References:

- Beinsteiner Brice., Klaholz Bruno., (2013) IBiSS, a versatile and interactive tool for integrated sequence and 3D structure analysis
- Clamp,M., Cuff,J., Searle,S.M. and Barton,G.J. (2004) The Jalview Java alignment editor. Bioinformatics, 20, 426–427.
- Waterhouse, A.M., Procter, J.B., Martin, D.M.A., Clamp, M. and Barton, G.J. (2009) Jalview Version 2--a multiple sequence alignment editor and analysis workbench. Bioinformatics, 25, 1189–1191.
- Herráez, A. (2006) Biomolecules in the computer: Jmol to the rescue. Biochem. Mol. Biol. Educ. Bimon. Publ. Int. Union Biochem. Mol. Biol., 34, 255–261.
- Cammer,S. (2007) SChiSM2: creating interactive web page annotations of molecular structure models using Jmol. Bioinformatics, 23, 383–384.