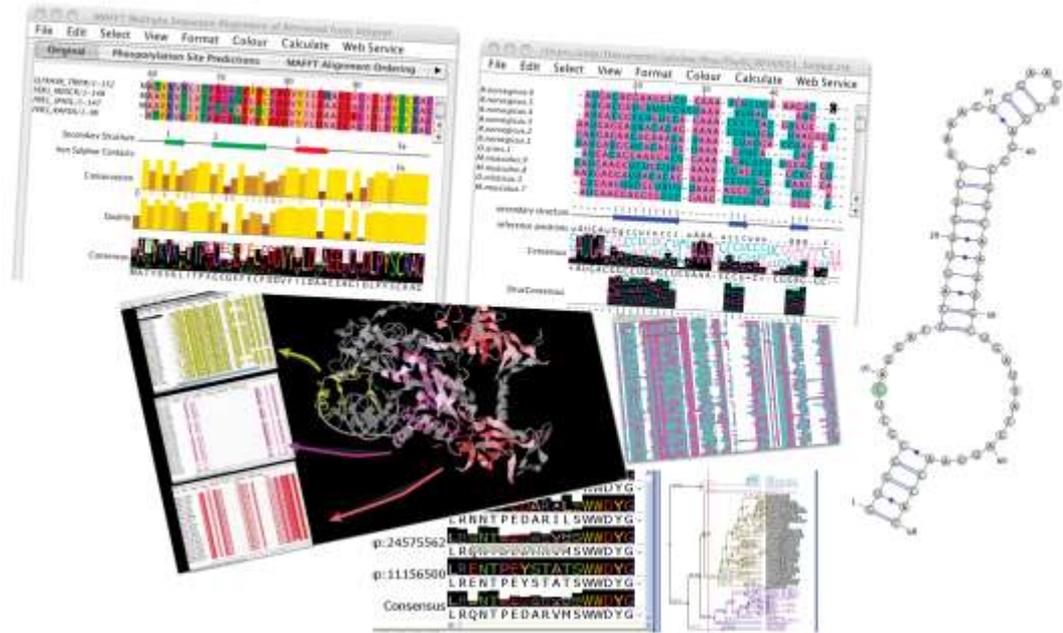


Practical Jalview



Jim Procter
University of Dundee
24th October 2014

supported by
wellcome trust



THE BARTON GROUP



9.00-9.15am.

Overview of the day

9.15am - 10.30am.

Session 1. Introduction to Jalview

- starting the application, importing alignments, basic editing and creating figures.

10.30-11am.

Coffee

11am - 12.30pm.

Session 2: Alignment & alignment analysis

- Creating sequence alignments, importing and calculating trees, tree based alignment analysis

12.30pm to 1.30pm.

Lunch

1.30pm – 3.00pm.

Session 3: Annotating sequences & alignments

- Creating and viewing sequence annotation
- Protein Secondary structure prediction

3.00pm – 3.30pm

Coffee

3.30pm – 4.30pm.

Session 4: Working with molecular structures

- Viewing 3D Structures, superimpositions, mapping disorder and alignment quality
- Viewing RNA Secondary Structure

4.30pm – 4.45pm.

Wrapup – what we didn't cover today

Course materials

Everything (will be) online

<http://www.jalview.org/tutorial/training-materials/2014/Dundee/Oct/>

- These slides**
- Jalview v2.8 Manual (v1.4.1)**
 - Log in and**
 - Open the manual in your PDF Viewer NOW**
- Additional exercises + ‘advanced topics’**



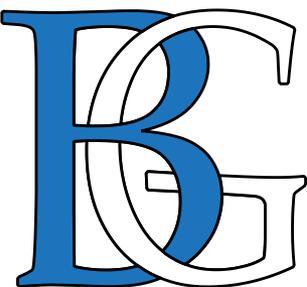
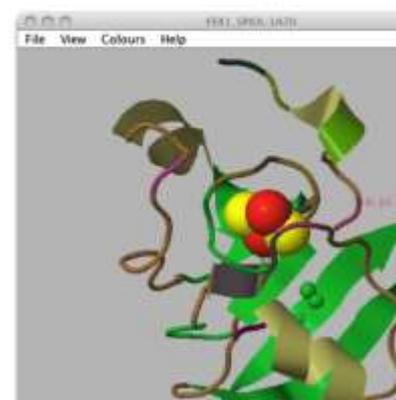
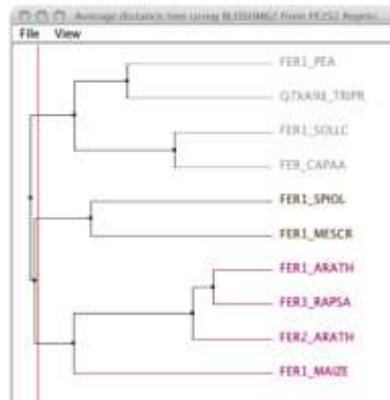
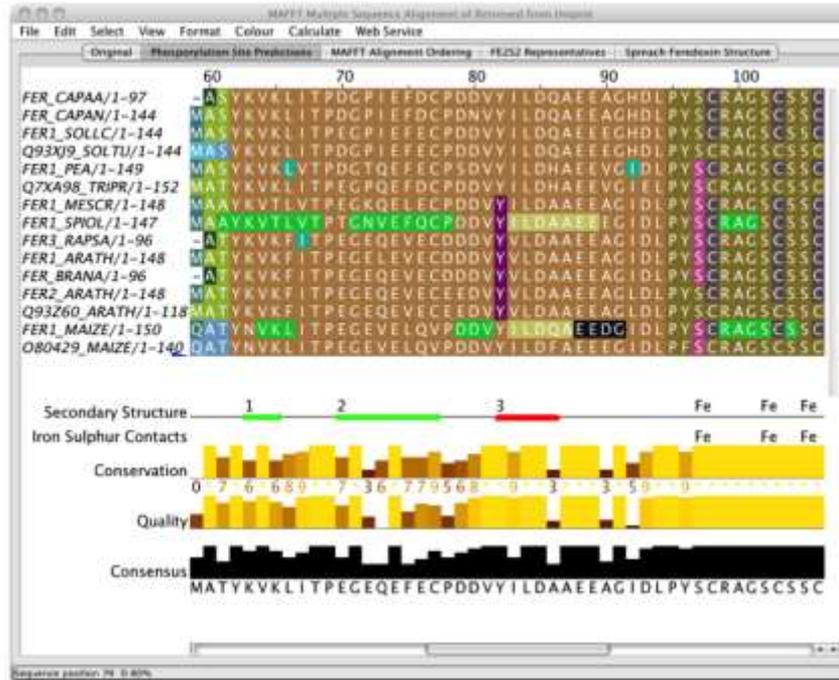
Java

Standalone or web based

alignment & annotation, tree, and structure **viewer** and editor

Available at

www.jalview.org



THE BARTON GROUP



www.compbio.dundee.ac.uk

Jalview
Launch
Buttons

Launch Jalview Applet

Launch Jalview Desktop

Home About Help Community Development Training Download

Latest News

Jalview in 2017
2013

Posted On: 10-01-2017

Help and
documentation

the new look

www.jalview.org

Posted On: 12-11-2012

GENERAL

Registration now open
for 3rd Jalview
Residential Training
Course and Hackathon

Posted On: 19-10-2012

TRAINING

Jalview is a free program for multiple sequence alignment editing, visualisation and analysis. Use Jalview to view and edit sequence alignments, analyse them using phylogenetic trees and principal component analysis (PCA) plots and explore molecular structure and annotation.

The Jalview Desktop

Jalview
training news
and course
dates

Installation
packages
and source

Jalview
Community

Jalview
Development and
release history

Analysis Services



Biological
Data
Services



The Jalview

Javascript API



applet
parameters

Alignment
And
Annotation

<http://www.jalview.org>

Jalview comes in two flavours

Launch Jalview Applet

Launch Jalview Desktop

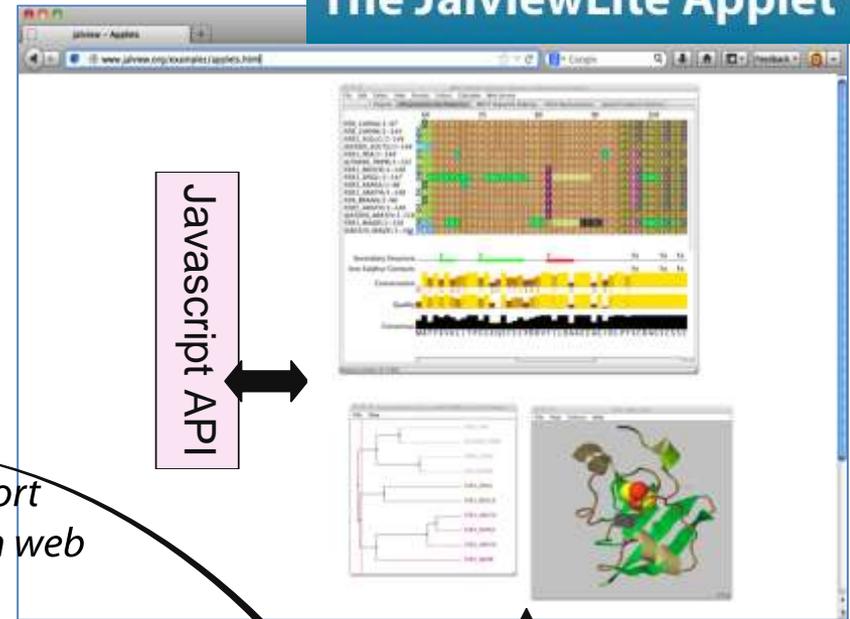
The Jalview Desktop



Analysis Services

Biological Data Services

The JalviewLite Applet



import from web

applet parameters

Alignment And Annotation

Bioinformatics Web Server

Ex 1 – starting The Jalview Dekstop

PAGE 7

Use the ‘Latest Build of Current Release’
via the development page

<http://www.jalview.org/development/development-builds>

Webstart launch link is

http://www.jalview.org/builds/release/webstart/jalview_2G.jnlp

Launching the jalview desktop

Jalview 2.8

The screenshot displays the Jalview desktop application interface. The main window, titled "MAFFT Multiple Sequence Alignment of Retrieved from Uniprot", shows a sequence alignment of several proteins. The alignment is color-coded by amino acid type. The proteins listed are Q7XA98_TRIPR/1-152, FER1_MESCR/1-148, FER1_SPIOL/1-147, FER3_RAPSA/1-96, FER1_ARATH, FER_BRU, FER2_A, Q93260, and FER1_MAIZE. A secondary window titled "Average distance tree using B..." shows a phylogenetic tree with the same protein names as labels. In the foreground, a splash screen for Jalview 2.8.0b1 is displayed, featuring the Jalview logo and the following text:

Version: 2.8.0b1

Last Updated: 31 January 2014
...Checking latest version...
Authors: Jim Procter, Andrew Waterhouse, Jan Engelhardt, Lauren Lui, Michele Clamp, James Cuff, Steve Searle, David Martin & Geoff Barton
Development managed by The Barton Group, University of Dundee, Scotland, UK.

For help, see the FAQ at www.jalview.org and/or join the jalview-discuss@jalview.org mailing list
If you use Jalview, please cite:
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 doi: 10.1093/bioinformatics/btp033



Jmol

Jalview 2.8

MAFFT Multiple Sequence Alignment of Retrieved from Uniprot

File Edit Select View Format Colour Calculate Web Service

Original

Spinach Ferredoxin Structure

FE2S2 Representat

	60	70	80	90	100
Q7XA98_TRIPR/1-152	MATYKVKLITPEGPOE	EFCPDDVYILDHAE	EEVGIELPYSCRAG	SCSS	
FER1_MESCR/1-148	MAAYKVTLVTP	EGKQEELECPDDVY	ILDAAEEAGIDL	PYSCRAGSCSS	
FER1_GNLC/1-148	MAAYKVTLVTP	EGKQEELECPDDVY	ILDAAEEAGIDL	PYSCRAGSCSS	

Average distance tree using B...

File View



Jalview Usage Statistics



Do you want to help make Jalview better by enabling the collection of usage statistics with Google Analytics ?

(you can enable or disable usage tracking in the preferences)

Cancel

No

Yes



Sequence position 87 11.0



Jmol

Jalview News

MATYKVKLITPEGPEFDCPDDVYILDHAEVGIELPYSCRAGSCSS

News from www.jalview.org

brought to you by JSwingReader (jswingreader.sourceforge.net)

- Jan 4, 2013 Jalview in 2012 and 2013
- Nov 12, 2012 Jalview 2.8 release and the new look www.jalview.org
- Oct 18, 2012 Registration now open for 3rd Jalview Residential Training Course and
- Sep 22, 2011 Welcome to the Jalview Desktop news channel

Jalview in 2012 and 2013

<http://www.jalview.org/General/General-news/Jalview-in-2012-and-2013>

2012 was quite a year here at jalview.org. A number of long running projects finally bore fruit with the launch of our new website and logo, and the release of [Jalview Version 2.8](#). The November release of Jalview was the first to support [JABAWS 2](#), which was launched in December 2011, and to include RNA visualization features developed by our 2010 and 2011 Google Summer of Code students: Lauren Lui and Jan Engelhart.

<http://www.jalview.org/feeds/desktop/rss>

Database Fetchers

Anatomy of Jalview: Figure 1.7

The image displays the Jalview 2.4 (pre) Desktop Window, which is divided into several functional areas:

- Desktop Window:** The main application window with a menu bar (File, Tools, Vamsas, Help, Window) and a title bar (Jalview 2.4 (pre)).
- Alignment Window:** The central workspace for sequence alignment, titled "MAFFT Multiple Sequence Alignment of Retrieved from Uniprot". It features a menu bar (File, Edit, Select, View, Format, Colour, Calculate, Web Service) and tabs for "Original", "Spinach Ferredoxin Structure", "FE2S2 Representatives", and "MAFFT Alignment Ordering".
 - Alignment View Tabs:** Located at the top left of the alignment window.
 - Sequence ID Panel:** A list of sequence identifiers on the left side, including FER1_PEA/1-149, Q7XA98_TRIPR/1-152, FER1_MESCR/1-148, FER1_SPIOL/1-147, FER1_BRANA/1-96, FER2_ARATH/1-148, Q93Z60_ARATH/1-118, FER1_MAIZE/1-150, and O80429_MAIZE/1-140.
 - Sequence Alignment:** A multi-colored grid representing the alignment of amino acid residues across the sequences.
 - Alignment Ruler:** A horizontal scale at the top of the alignment grid, with markers at 70, 80, 90, and 100.
 - Alignment Annotation:** A series of horizontal bars below the alignment grid, including "Secondary Structure" (with green and red arrows), "Iron Sulphur Contacts" (with "Fe" labels), "Conservation" (yellow and brown bars), "Quality" (yellow and brown bars), and "Consensus" (black bars).
 - Annotation Label Panel:** A panel on the left side of the alignment window.
 - Alignment Scrollbar:** A vertical scrollbar on the right side of the alignment grid.
 - Status bar:** Located at the bottom of the alignment window, displaying "Sequence 4 ID: Q93XJ9_SOLTU Residue: GLY (79)".
 - Ruler Scrollbar:** A horizontal scrollbar at the bottom of the alignment window.
- Tree Window:** A separate window titled "Average distance tree using BLO..." showing a phylogenetic tree with branches and labels for sequences like FER1_PEA, Q7XA98_TRIPR, FER1_SPIOL, FER1_MESCR, FER1_ARATH, FER3_RAPSA, FER2_ARATH, and FER1_MAIZE.
- Structure Window:** A window titled "FER1_SPIOL:1-147" showing a 3D ribbon structure of the protein. It includes a menu bar (File, View, Colours, Help) and a label "HR 89" with a distance of "1.325 nm". The Jmol logo is visible in the bottom right corner.

Ex 1 – starting Jalview

- Tasks

- Modify user preferences
- Test that you can load the example file manually

http://www.jalview.org/examples/exampleFile_2_7.jar

Ex 1 – starting Jalview

- Tasks

- Modify user preferences
- Test that you can load the example file manually

http://www.jalview.org/examples/exampleFile_2_7.jar

- Questions

- Where to find help ?
- How to report a bug ?

Jalview Community

- Mailing lists
 - Discussion forum and developers forum
 - Links from <http://www.jalview.org/community>
- Jalview bug database
 - <http://issues.jalview.org>
 - Also indexed on google
- Jalview development info
 - <http://www.jalview.org/development>

Ex 2 - Navigation

- Tasks
 - Open the overview window for a view
 - Jump to a specific row and column with keyboard mode

Ex 2 - Navigation

- Tasks
 - Open the overview window for a view
 - Jump to a specific row and column with keyboard mode
- Questions
 - How do you locate a sequence or sequence position if you don't know its row/column ?
 - How do you find a sequence motif ?

Ex 3 Getting data into Jalview

- Tasks
 - Importing an alignment via a url, local file, or cut' n' paste
 - Getting an alignment from Pfam

Ex 3 Getting data into Jalview

- Tasks
 - Importing an alignment via a url, local file, or cut' n' paste
 - Getting an alignment from Pfam
- Questions
 - What happens when you drag a file onto an existing alignment ?
 - What is different about the alignment retrieved from Pfam ?
 - What if you want to load a *really* big alignment ?

Ex 4. Saving alignments

- Tasks
 - Save alignments in different formats

Ex 4. Saving alignments

- Tasks
 - Save alignments in different formats
- Questions
 - What's the biggest difference between a BLC file and a pileup file ?
 - Why are Jalview projects useful ?

Ex 5,6,7,8 and 9

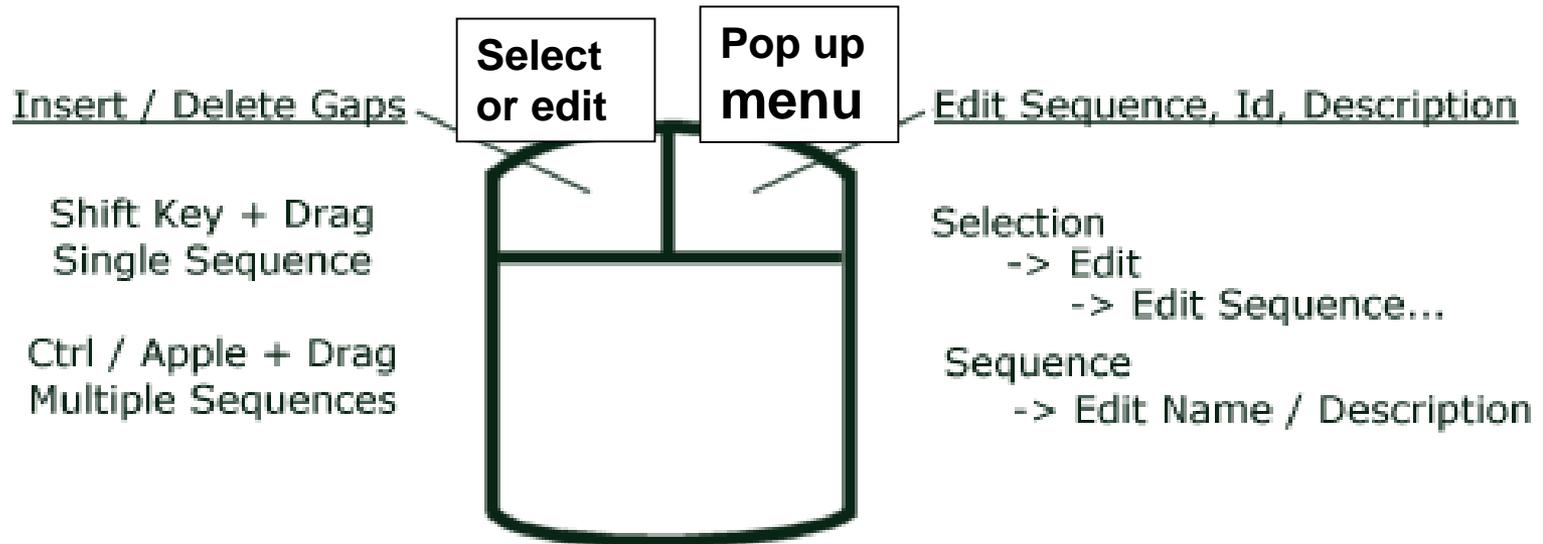
selecting, reordering,

hiding/showing and editing

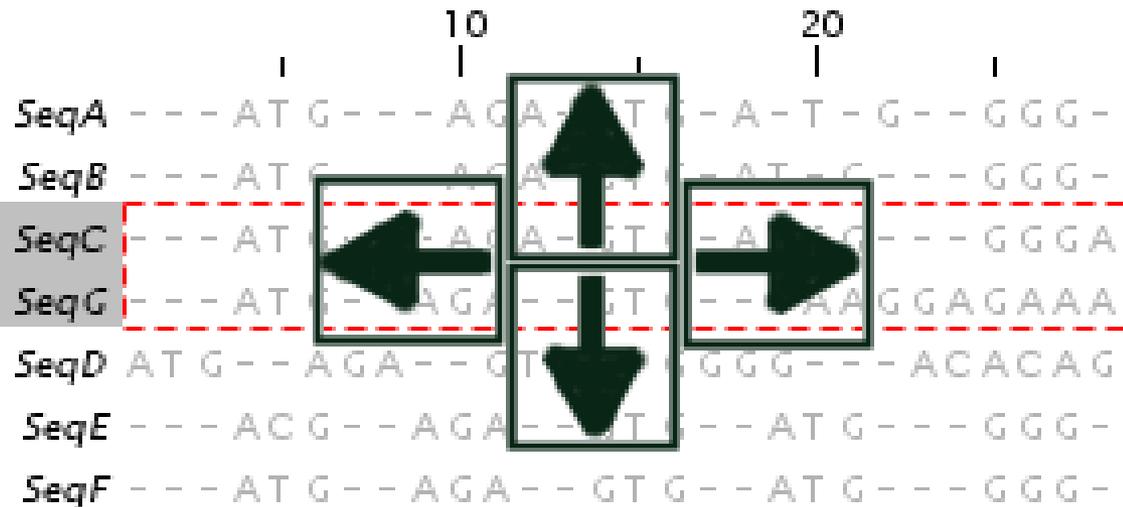
- Tasks
 - Get used to the mouse and keyboard based selection and alignment editing controls
 - Learn how to work on specific parts of an alignment
- Exercise 8 and 9 let you practice mouse and keyboard based editing techniques
 - If you don't finish them now, do them when you have a spare 15 mins at lunch.

How do I edit sequences in Jalview

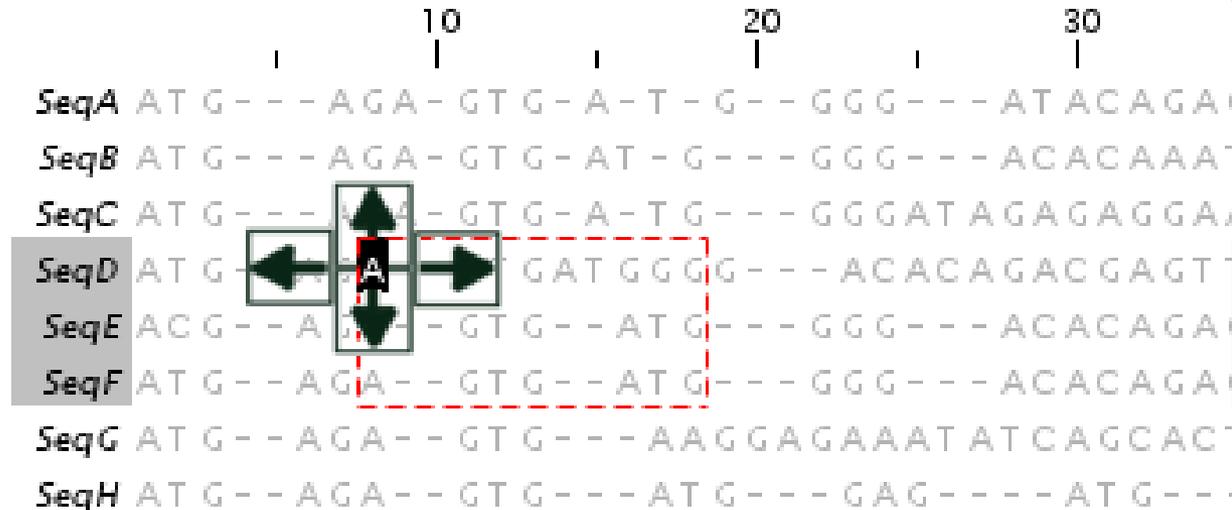
<http://www.jalview.org/examples/editing.html>



Selected sequences can be moved up and down or slid from left to right



F2 enables/disables keyboard mode



Cursor Keys - Move Cursor

Alt + Cursor Keys - Move Sequence

[X] Space - Insert [X] gap(s)

[X] Delete / Backspace - Delete [X] gap(s)

8 C - Move to Column 8

4 S - Move to Sequence 4

8,4<return> - Move to column 8, sequence 4

6 P - Move to Position 6

Q - Define the top left corner of selection area

M - Define the bottom right corner of selection area

Windows 7 Users:

Group Insert - use

Shift+Space

(not CTRL+Space)

Ex 5,6,7,8 and 9

selecting, reordering, hiding/showing and editing

- **Tasks**
 - Get used to the mouse and keyboard based selection and alignment editing controls
 - Learn how to work on specific parts of an alignment
- **Questions**
 - Why would you create representative sequences ?
 - How do you insert a gap in the middle of a sequence without affecting the rest of its alignment ?

Ex 10 & 11 : Colouring

- Tasks
 - Learn how to colour all, or part of the alignment by
 - Amino acid property
 - Annotation

Ex 10 & 11 : Colouring

- Tasks

- Learn how to colour all, or part of the alignment by

- Amino acid property
 - Annotation

- Questions

- Why is colouring the alignment useful ?

- How would you highlight acidic residues in your alignment ?

Ex 12,13 – alignment layout and export

- Tasks
 - Adjust the alignment formatting options
 - Wrap
 - Sequence id margin
 - Export the alignment as a figure
 - HTML, EPS and PNG

Ex 12,13 – alignment layout and export

- Tasks
 - Adjust the alignment formatting options
 - Wrap
 - Sequence id margin
 - Export the alignment as a figure
 - HTML, EPS and PNG
- Questions
 - How do you control the number of columns shown in wrapped mode ?
 - How can you easily experiment with different alignment figure layouts ?
 - What programs can edit EPS files ?

- End of Session 1
 - Loading/saving
 - Navigation/Editing
 - Colouring & Figures

- Session 2
 - Alignment with JABAWS
PAGE 58 IN MANUAL
 - Alignment analysis
 - Trees
 - PCA
 - Subfamily analysis

Anatomy of Jalview: Figure 1.7

The image displays the Jalview 2.4 (pre) software interface, which is used for multiple sequence alignment and visualization. The main window is titled "Alignment Window" and shows a MAFFT Multiple Sequence Alignment of Retrieved from Uniprot. The alignment is displayed in a color-coded format, with a ruler at the top indicating residue positions (70, 80, 90, 100). The alignment is annotated with secondary structure elements (green arrows) and iron-sulphur contacts (red bars). Below the alignment, there are conservation, quality, and consensus tracks. The status bar at the bottom indicates the sequence ID: Q93XJ9_SOLTU and the residue: GLY (79).

Key components of the interface are labeled:

- Desktop Window:** The top window showing the operating system environment.
- Alignment Window:** The main window displaying the sequence alignment.
- Alignment View Tabs:** Tabs for "Original", "Spinach Ferredoxin Structure", "FE2S2 Representatives", and "MAFFT Alignment Ordering".
- Sequence ID Panel:** A list of sequence identifiers on the left side of the alignment window.
- Alignment Ruler:** A horizontal scale at the top of the alignment window showing residue positions.
- Alignment Annotation:** Tracks for secondary structure, iron-sulphur contacts, conservation, quality, and consensus.
- Alignment Scrollbar:** A vertical scrollbar on the right side of the alignment window.
- Annotation Label Panel:** A panel on the left side of the alignment window for labeling annotations.
- Status bar:** A bar at the bottom of the alignment window showing the current sequence ID and residue.
- Ruler Scrollbar:** A horizontal scrollbar at the bottom of the alignment window.
- Tree Window:** A window showing a phylogenetic tree of the sequences.
- Structure Window:** A window showing a 3D ribbon diagram of the protein structure, with iron atoms (Fe) and sulphur atoms (S) highlighted.

Clustal Omega quick alignment of millions of sequences



Assorted protein disorder predictors



Protein conservation calculations



File Edit Search Home Calculator Web Service

- Alignment ▶
- Secondary Structure Prediction ▶
- Protein Disorder ▶
- Analysis ▶
- Conservation ▶
- Envision 2 ▶
- Fetch DB References ▶

www.compbio.dundee.ac.uk/jabaws

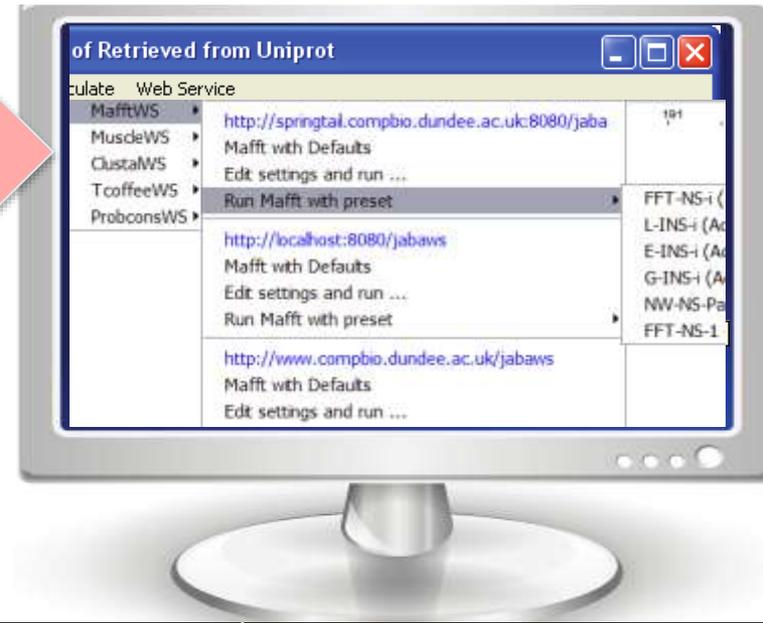
JABAWS:MSA Troshin et al. 2011,
Bioinformatics.

JABAWS 2 In Preparation.



Jalview Web
Service GUI

JABAWS
Java Client



JABAWS Virtual
Appliance for
your private use.



Native JABAWS installs
on a range of platforms



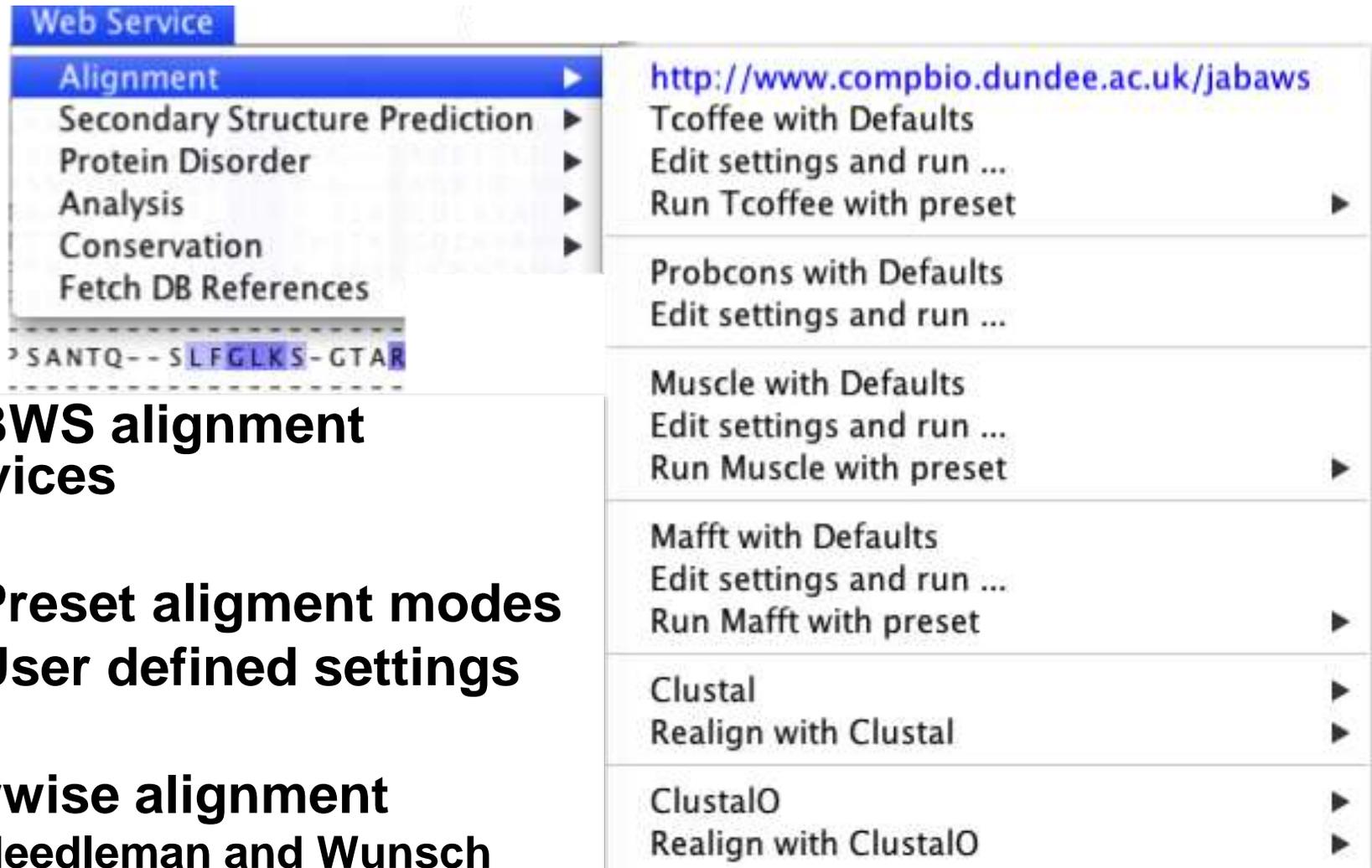
Apache
Tomcat



JABAWS Amazon
Machine Image
on EC2



Jalview's Alignment Methods

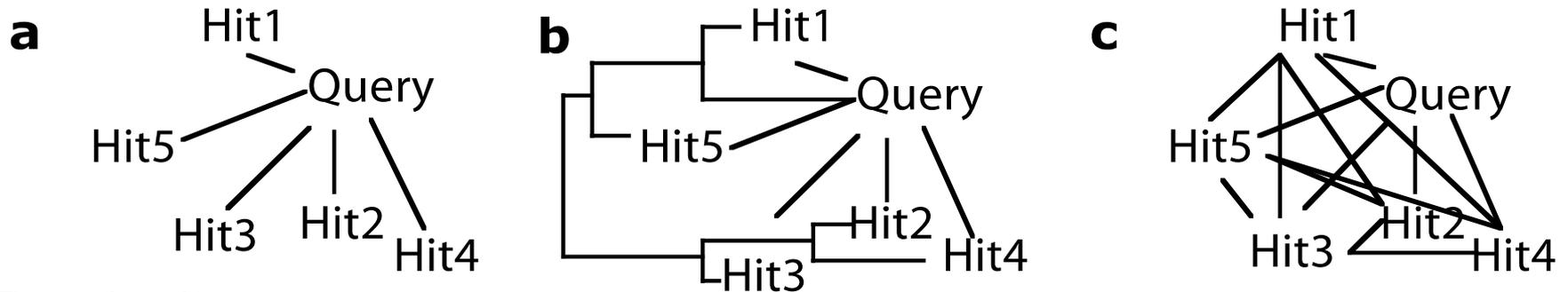


The screenshot shows the 'Web Service' menu in Jalview. The 'Alignment' option is selected, revealing a list of alignment methods. Each method includes an option to 'Edit settings and run ...' and a 'Run' option with a preset. The methods listed are: Tcoffee with Defaults, Probcons with Defaults, Muscle with Defaults, Mafft with Defaults, Clustal, and ClustalO. The sequence 'SANTQ--SLFGLKS-GTAR' is visible at the bottom of the menu.

Method	Options
http://www.compbio.dundee.ac.uk/jabaws	Tcoffee with Defaults Edit settings and run ... Run Tcoffee with preset
Probcons with Defaults	Edit settings and run ...
Muscle with Defaults	Edit settings and run ... Run Muscle with preset
Mafft with Defaults	Edit settings and run ... Run Mafft with preset
Clustal	Realign with Clustal
ClustalO	Realign with ClustalO

- **JABWS alignment services**
 - Preset alignment modes
 - User defined settings
- **Pairwise alignment**
 - Needleman and Wunsch
 - Mostly used internally

Common types of alignment algorithm



- Sequence database searches – optimal alignment between query and hit
e.g. **Blast** (single sequence), **PSI-Blast** and **HMMER**
- Progressive – optimise alignment between branches on guide tree
e.g. **ClustalW**
- Transitive – optimise MSA to maximise consistency between pairs
e.g. **T-COFFEE**, **ProbCons**

Profile methods – e.g. Muscle and MAFFT are hybrid of **b** and **c**.

Latest methods, e.g. **ClustalO**, also employ sampling strategies to speed up tree building & refinement.

Jalview alignment exercise 25 (sect. 2.4)

- Tasks
 - Align sequences using different methods
 - Use the Webservices' 'alignment' submenu
 - Explore how hidden regions affect alignment jobs.

Jalview alignment exercise 25 (sect. 2.4)

- Tasks
 - Align sequences using different methods
 - Use the Webservices' 'alignment' submenu
 - Explore how hidden regions affect alignment jobs.
- Questions
 - Why does jalview run several jobs if the input includes hidden regions ?
 - What does 're-alignment' mean ?

LUNCH

Alignment Job Parameter Settings

The image shows a software dialog box titled "Edit parameters for Align with MuscleWS". The dialog is divided into several sections: "Details", "Options", and "Parameters".

- Details:** A text box for adding notes.
- Options:** A list of checkboxes including "dimer", "Diagonal", "Diagonal 1", and "Profile scoring method" (which is checked).
- Parameters:** A section for "Sequence type" with a dropdown menu set to "auto".

Callout boxes provide the following information:

- "Browse or edit to change name of set" points to the "Current parameter set name" dropdown menu.
- "Buttons appear to create, update, rename or delete user settings." points to the "Revert" and "Create" buttons.
- "text box to add notes for the parameter set" points to the text box in the "Details" section.
- "Parameters contains more complex settings" points to the "Parameters" section.
- "Start job with current settings or cancel." points to the "Start Job" and "Cancel Job" buttons at the bottom.
- "Tooltips give brief description and link (right click) to further info" points to a tooltip for the "Profile scoring method" option, which reads: "le - use log-expectation profile score VTML240 (default sequences.) sp - use sum-of-pairs protein profile score use sum-of-pairs profile score (VTML240) [Link](#)".

Why change alignment
parameters ?

Jaba Alignment Exercise

- Task
 - Run the alignment from step **b** of ex. 25 using the JABA clustalW service
 1. Run with default settings
 2. Use the ‘Edit parameters’ dialog to run an alignment with the following:
 - Gap opening (internal and end gaps) = 3
 - Gap Extension = 0.05
 - Compare the two alignments. You may want to save them for later, too.
- Questions
 - What effect has modifying the gap penalties had on the ferredoxin alignment ?

- Session 2
 - Alignment with JABAWS
 - PAGE 58 IN MANUAL***
 - Alignment analysis
 - Trees
 - PCA
 - Subfamily analysis

Alignment analysis – Section 2.2

- Principal component analysis
- Phylogenetic trees
- Redundancy removal
- Tree based conservation analysis
- Subdividing alignment by mutation

Phylogenetic analysis and Jalview

- Built in tree methods
 - UPGMA
 - Fast, simple, but not reliable for phylogenetic inference
 - Neighbour joining
 - Slower than UPGMA
 - Useful for a first approximation
 - NJ does not work well for very divergent sequence sets
 - » Need to add in close relatives to get an idea of topology
- Import trees from elsewhere
 - Load a Newick format tree file onto an alignment from another program

PCA and Phylogeny Section 2.2

Exercise 17 and 18

- Tasks
 - Calculate Principal component analyses (PCAs) and trees on the ferredoxin alignment
 - Explore the use of the interactive tree viewer
 - Use it to select subgroups on the alignment.

PCA and Phylogeny Section 2.2

Exercise 17 and 18

- Tasks
 - Calculate Principal component analyses (PCAs) and trees on the ferredoxin alignment
 - Explore the use of the interactive tree viewer
 - Use it to select subgroups on the alignment.
- Questions
 - What is the role of BLOSUM62 or Percentage identity in the tree building process ?

Tree based conservation analysis

Sect. 2.2.3 Exercise 19

- “Poor man’ s” character inference analysis
 - Compare conservation patterns within and between branches of a tree
- Task
 - Use interactive tree viewer to subdivide alignment and identify difference in conservation pattern

Tree based conservation analysis

Sect. 2.2.3 Exercise 19

- “Poor man’ s” character inference analysis
 - Compare conservation patterns within and between branches of a tree
- Task
 - Use interactive tree viewer to subdivide alignment and identify difference in conservation pattern
- Questions
 - How can you tell which differences are important ?

Sub-groups and Sub-group Annotation

Exercise 21

- Task
 - Use the group consensus sequence logos to more easily compare tree subgroups
 - Use ‘Make groups for selection’ to subdivide groups by specific mutation

Sub-groups and Sub-group Annotation

Exercise 21

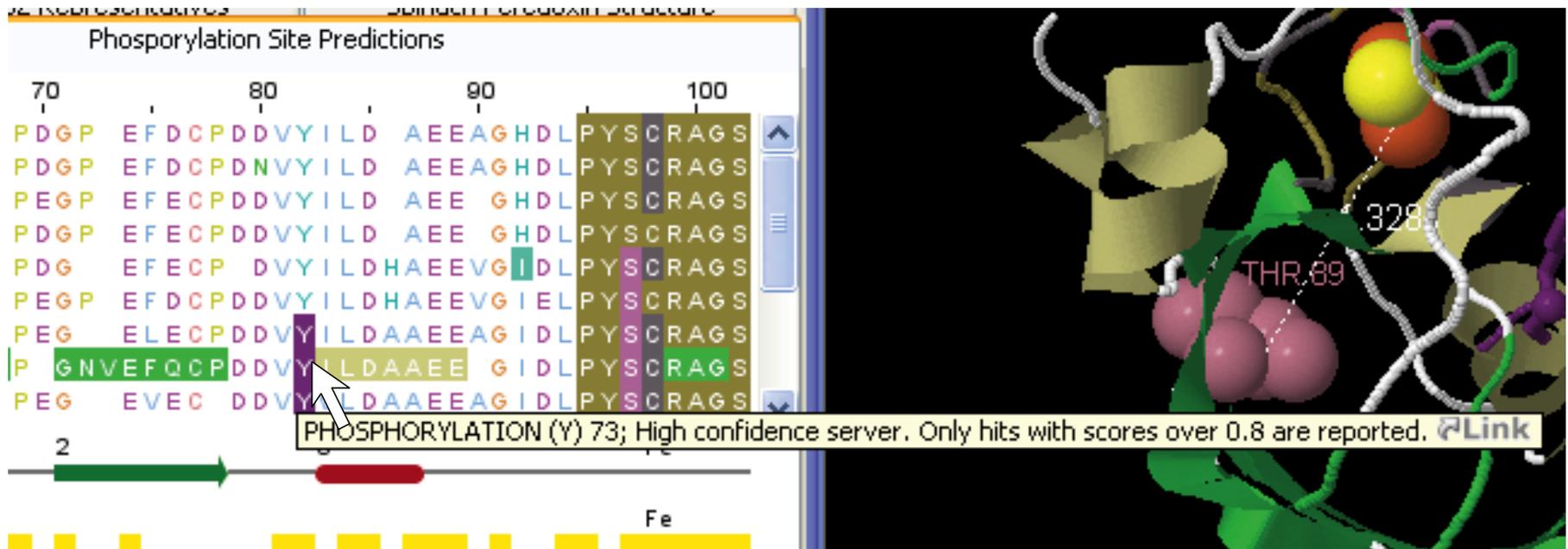
- Task
 - Use the group consensus sequence logos to more easily compare tree subgroups
 - Use ‘Make groups for selection’ to subdivide groups by specific mutation
- Questions
 - How can you navigate the sub-groups of a large alignment ?

- End of Session 2
 - Alignment & analysis

- Session 3
 - Sequence DB refs and Sequence Features
 - Protein secondary structure prediction

Sequence Features

Manual section 2.8



Getting and working with sequence features and annotation

- Sequence Databases
- Sequence feature sources
 - DAS Sequence feature retrieval
 - GFF and Jalview feature files
- Visualizing features
 - Highlighting annotated regions
 - Shading and reordering based on scores and labels

```

P17870 P - - P N L - P C S V T L Q P G P E D T G K A
P51485 A - - P K S - A S S V T L Q P A P G D T G K F
P51466 P - - Q N L - P C S V T L Q P G P E D T G K A
P51487 P - - P N S - P S S V T L Q Q E G D D L G K F
P51477 P - - D F L - P C S V S L Q P A P S D V G K A
P51484 P - - E N A - P P S V T L Q P G S E D Q G R F
P32122 P - - A S S - P S S V T L Q P G D D D Q G K F
P08168 P - - D Y L - P C S V M L Q P A P Q D V G K S
P53179 P R G R G M - L S S I - - - - - - - - K F E F
Q09889 P - - P D I - P D S I - - - - - - - - E G I F
P30647 P - - L N C - P S S Y - - - - - - - - E S Q F
O45782 P - - K S L - P S S F - - - - - - - - E G E F
O76685 P - - I N V - P P S F - - - - - - - - E G K F
O17812 P - - E N I - P Q S F - - - - - - - - E G P F

```

Sequence Feature Settings

Feature Settings
DAS Settings

uniprot
 PDBsum_protprot

Pfam Other Features
 cbs_total

Feature Type	Colour	Display
DISULFID	<div style="width: 20px; height: 10px; background-color: #0056b3;"></div>	<input checked="" type="checkbox"/>
Protein-protein contact	<div style="width: 20px; height: 10px; background-color: #6a3d9a;"></div>	<input checked="" type="checkbox"/>
MOD_RES	<div style="width: 20px; height: 10px; background-color: #00ff00;"></div>	<input checked="" type="checkbox"/>
ISOFORM	<div style="width: 20px; height: 10px; background-color: #4b2c2c;"></div>	<input checked="" type="checkbox"/>
PHOSPHORYLATION (S)	<div style="width: 20px; height: 10px; background-color: #c06090;"></div>	<input checked="" type="checkbox"/>
PHOSPHORYLATION (Y)	<div style="width: 20px; height: 10px; background-color: #6a3d9a;"></div>	<input checked="" type="checkbox"/>
INIT_MET	<div style="width: 20px; height: 10px; background-color: #bcb87d;"></div>	<input checked="" type="checkbox"/>
PHOSPHORYLATION (T)	<div style="width: 20px; height: 10px; background-color: #c06090;"></div>	<input checked="" type="checkbox"/>
NES-SIGNAL	<div style="width: 20px; height: 10px; background-color: #000080;"></div>	<input checked="" type="checkbox"/>
CONFLICT	<div style="width: 20px; height: 10px; background-color: #c04040;"></div>	<input checked="" type="checkbox"/>
ACETYLATION	<div style="width: 20px; height: 10px; background-color: #000080;"></div>	<input checked="" type="checkbox"/>
TURN	<div style="width: 20px; height: 10px; background-color: #000000;"></div>	<input checked="" type="checkbox"/>
HELIX	<div style="width: 20px; height: 10px; background-color: #bcb87d;"></div>	<input checked="" type="checkbox"/>
STRAND	<div style="width: 20px; height: 10px; background-color: #00ff00;"></div>	<input checked="" type="checkbox"/>
SIGNAL	<div style="width: 20px; height: 10px; background-color: #add8e6;"></div>	<input checked="" type="checkbox"/>
COMPBias	<div style="width: 20px; height: 10px; background-color: #800000;"></div>	<input checked="" type="checkbox"/>
PROSITE	<div style="width: 20px; height: 10px; background-color: #8b4513;"></div>	<input checked="" type="checkbox"/>
PRINTS	<div style="width: 20px; height: 10px; background-color: #8b4513;"></div>	<input checked="" type="checkbox"/>
PROPEPTIDE	<div style="width: 20px; height: 10px; background-color: #bcb87d;"></div>	<input type="checkbox"/>
OUTSIDE	<div style="width: 20px; height: 10px; background-color: #00ff00;"></div>	<input type="checkbox"/>
CHAIN	<div style="width: 20px; height: 10px; background-color: #9370db;"></div>	<input type="checkbox"/>
Pfam	<div style="width: 20px; height: 10px; background-color: #e91e63;"></div>	<input type="checkbox"/>
ProDom	<div style="width: 20px; height: 10px; background-color: #90ee90;"></div>	<input type="checkbox"/>

Invert Selection

OK

Cancel

Load Colours

Save Colours

Sequence Features

Section 2.8.1-3 & Ex 27

- Annotate the whole or part of a sequence
- Database refs are special case.
- Tasks
 - Visualise, create, modify, import and export features.

Sequence Features

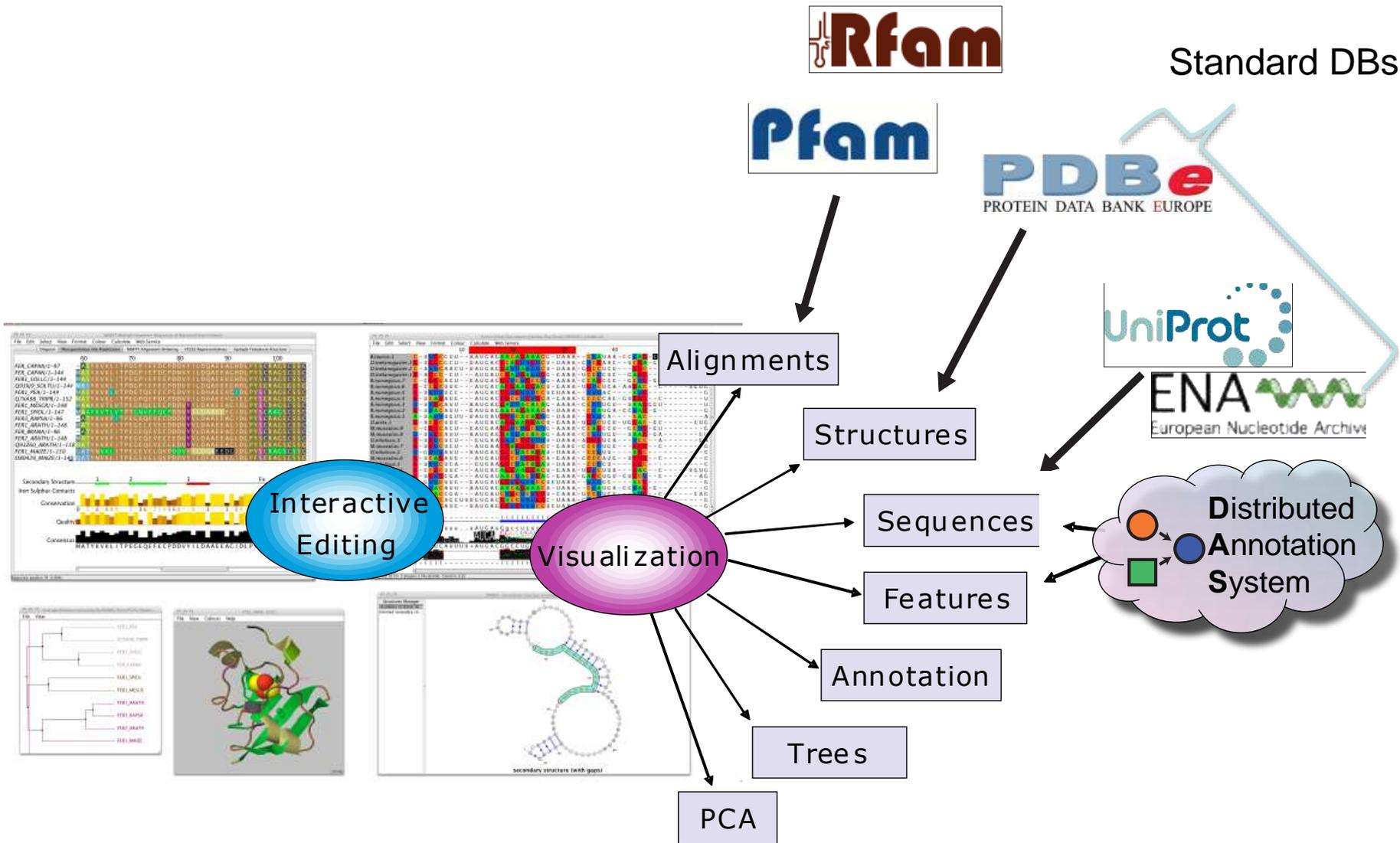
Section 2.6.1-3 & Ex 27

- Annotate the whole or part of a sequence
- Database refs are special case.
- Tasks
 - Visualise, create, modify, import and export features.
- Questions
 - What are the different types of file formats available for import and export
 - What services allow you to discover annotation for sequence ?

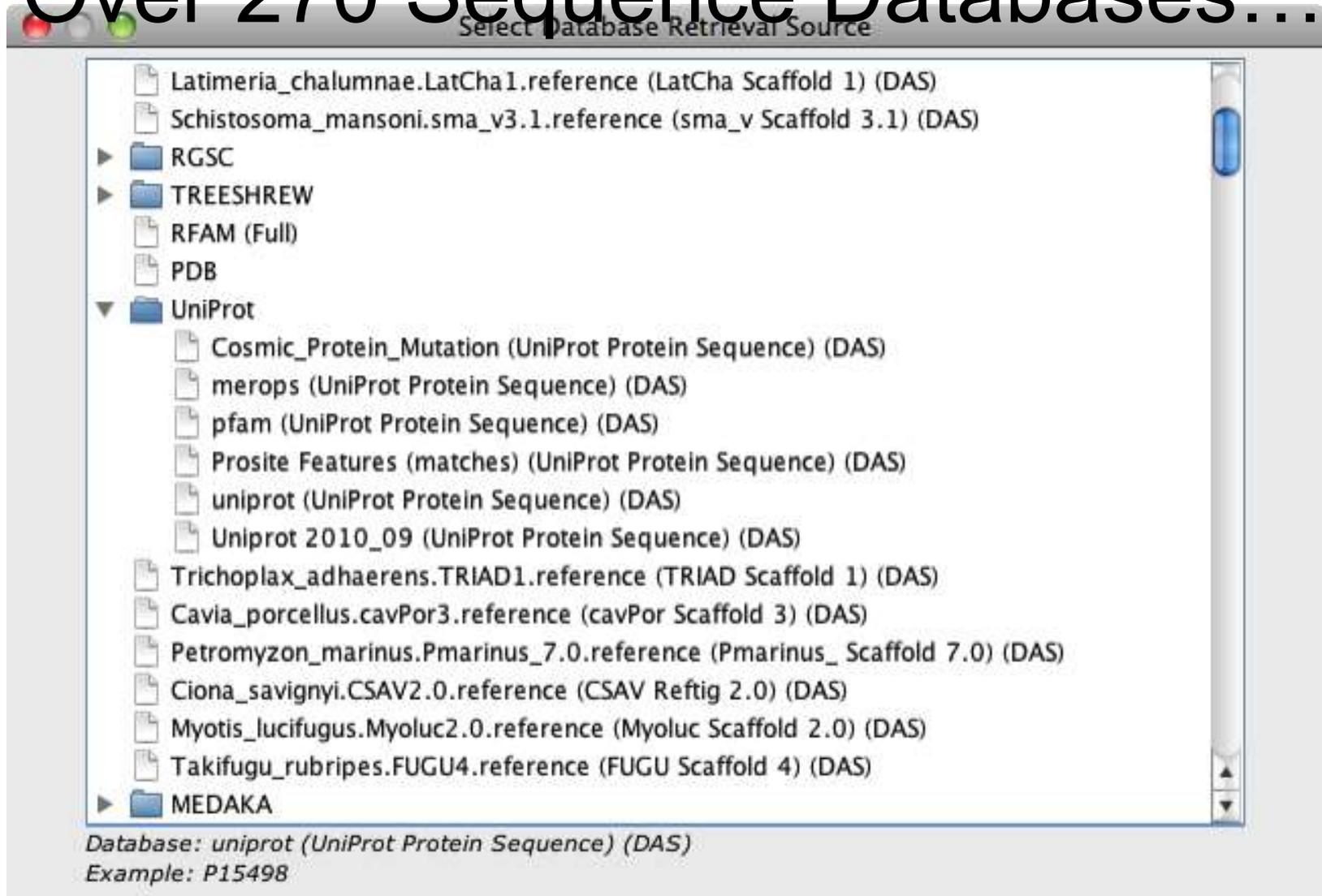
Sources of sequence feature data

- Jalview sequence annotation files
- DAS sources
- GFF files
- Certain 'rich' alignment formats
 - Stockholm
 - AMSA

Retrieval from External Databases



DAS allows Jalview access to Over 270 Sequence Databases...



Jalview and Sequence Databases

Sec 2.9.1 Ex. 29

- Can retrieve new sequences or match against existing records using IDs
- Task
 - Recover the Uniprot annotation for the ferredoxin sequences using their IDs
 - Verify retrieval by examining sequence annotation

Cut & Paste input - FASTA

File Edit Select View Format

Original View 1

UniProt/Swiss-Prot|P17870
 UniProt/Swiss-Prot|P51480
 UniProt/Swiss-Prot|P51460
 UniProt/Swiss-Prot|P51480
 UniProt/Swiss-Prot|P51470
 UniProt/Swiss-Prot|P51480
 UniProt/Swiss-Prot|P32120
 UniProt/Swiss-Prot|P08160
 UniProt/Swiss-Prot|P53170
 UniProt/Swiss-Prot|Q09880
 UniProt/Swiss-Prot|P30640
 UniProt/Swiss-Prot|O45780
 UniProt/Swiss-Prot|O76680
 UniProt/Swiss-Prot|O17810

Conservation

Quality

Consensus

Sequence 1 ID: UniProt/Swiss

Sequence Feature Settings

Feature Settings DAS Settings

Feature Settings	Us...	Nickname
Canis_familiaris....	<input type="checkbox"/>	
Canis_familiaris....	<input type="checkbox"/>	
Gallus_gallus.WA...	<input type="checkbox"/>	
Gallus_gallus.WA...	<input type="checkbox"/>	
Ornithorhynchus_...	<input type="checkbox"/>	
Ornithorhynchus_...	<input type="checkbox"/>	
Saccharomyces_c...	<input type="checkbox"/>	
Saccharomyces_c...	<input type="checkbox"/>	
Phobius	<input type="checkbox"/>	
uniprot	<input checked="" type="checkbox"/>	
cbs_total	<input type="checkbox"/>	
PDBsum_protpro...	<input type="checkbox"/>	
Pfam Other Feat...	<input type="checkbox"/>	

Nickname: uniprot
 URL: <http://www.ebi.ac.uk/das-srv/uniprot/das/aristotle/>
 Admin Email: uniprot-das@ebi.ac.uk
 Registered at: Sun Feb 11 17:15:51 GMT 2007
 Last successful test: Sun Feb 11 17:15:51 GMT 2007
 Labels: ENSEMBL, BioSapiens
 Capabilities: sequence, features, entry_points, stylesheet
 Coordinates: /coordsy

Authority: Any
 UniProt
 PDBresnum
 NCBI
 Ensembl
 SGD
 MOZ2a
 RGSC
 MGI

Clone	eFamily
Gene_ID	Predicted
Chromosome	ZFMODELS
Contig	Computationally inferred
Scaffold	eProtein
Volume Map	Manually curated

Use Registry

Find Uniprot Accession Ids

Do you want Jalview to find Uniprot Accession ids for given sequence names?

0

K A F C A E N L - -
 K T F V A V T D G -
 R A F C A K S I - -
 R A Y V A D S E - -
 K A F S T N N L - -
 K L F I A E T E - -
 K T W V G D H A - -
 K A F A T H S T D -
 S C T L E S L N N I
 T A S L E R A T Q -
 K V E L R A S T D -
 K A I C E R P W D -
 T A E V D R P W R -
 K V H M D R P H A -

4 5 1 4 3 2 3 3 0 -

The Distributed Annotation System

Section 2.9.2, Exercise 30

- Web servers that Jalview can use to discover annotation for a sequence
- Task
 - Browse available DAS sources for protein sequences
 - Retrieve annotation for the ferredoxin alignment.

The Distributed Annotation System

Section 2.9.2, Exercise 30

- Web servers that Jalview can use to discover annotation for a sequence
- Task
 - Browse available DAS sources for protein sequences
 - Retrieve annotation for the ferredoxin alignment.
- Question
 - What does the ‘optimise order’ button do ?

Working with sequence features

Ex 32 c,d,e (Sec 2.9.4 P. 80)

- Task
 - Shading features using labels and scores
 - Sorting alignment using feature scores

ONLY ATTEMPT: 32c, d, e

- DAS servers mentioned in exercise are not currently available
- Instead experiment with
 - Uniprot CHAIN annotation

Shading, thresholding, colour by label.

.. MASTALSSAIVSTSF LRRQQTPISLRSLPFANT.. QSLFGLKS
 .. MAATTTTMMGMATTFVPKPQAPPMM AALPSNTG.. RSLFGLKT
 .. MASISGTMISTSF LPRKPAVTS LKAIS.. NVG.. EALFGLKS
 .. MASTALSSAIVSTSF LRRQQTPISLRSLPFANT.. QSLFGLKS
 .. MASISGTMISTSF LPRKPVVTS LKAIS.. NVG.. EALFGLKS
 ATVLGSPRAPAFFSSSSSLRAAPAPTAVALPAAKVG... IMGRSA
 .. MASVSATMISTSFMPRKPAVTS LKPIP.. NVG.. EALFGLKS
 .. MATIPALYGTA VSTSFMR RQPVPMSVATT TTKAFPSGFG LKSV
 .. MAATTAALSGATMSTAFAPKT... PPMTAALPTNVG.. RALFGLKS
 .. MASTALSSAIVGTSF IRRSPAPISLRSLPSANT.. QSLFGLKS
 .. MAATALSMSILRAPP.. PCFSSPLRLRVAVAKPLAAMP
 .. MATIPALYGTA VSTSF LRTQPMPMSVTTTKAFSN.. GFLGLKT.. SLK

.. MMAS+ALSGT+VSTSF LRRQPAPTSLAALP+NVG.. +SLFGLKS.. STA

VYILDQAAEEAGHDL PYS CRAGSCSSCAGKIAGGAVDQTDGNFLDDQLE
 VYVLDAAEEAGLDPYS CRAGSCSSCAGKVVVSGSIDQSDQSFLDD...
 VYILDQAAEEEGIDL PYS CRAGSCSSCAGKLTGSLND...
 VYILDQAAEEEGHDL PYS CRAGSCSSCAGKVTAGSVDQSDGNFLDDEQEA
 VYVLDAAEEAGIDL PYS CRAGSCSSCAGKVVVSGSVDQSDQSFLDDQIA
 VYVLDAAEEAGLDPYS CRAGSCSSCAGKVVVSGSIDQSDQSFLDDEQMS
 VYILDQAAEEEGHDL PYS CRAGSCSSCAGKVTAGTVDDQSDKFLDDQEA
 VYILDQAAEEDGIDL PYS CRAGSCSSCAGKVVVSGSVDQSDQSYLDDGQIA
 VYILDQAAEEAGHDL PYS CRAGSCSSCAGKIAGGAVDQTDGNFLDDQLE
 VYILDHAAEEVGI ELPYS CRAGSCSSCAGKVVNGVNDQDGSFLDDEQIE
 VYVLDAAEEAGIDL PYS CRAGSCSSCAGKVVSGFVDQSDSFLDDQIA
 VYILDQAAEEAGIDL PYS CRAGSCSSCAGKVTSGSVNQDDGSFLDDQI
 VYVLDAAEEAGIDL PYS CRAGSCSSCAGKVVVSGSVDQSDQSFLDDEQIC
 VYILDFAEEEGIDL PYS CRAGSCSSCAGKVVVSGSVDQSDQSFLNDNQVA
 VYILDHAAEEVGI ELPYS CRAGSCSSCAGKVVGGVDDQSDGSFLDDEQIEAGFVLT CVAYPTSDVVVIE TH

Graduated Feature Colour for hydrophobic_region

Colour by Label Min: Max:

No Threshold Adjust threshold Threshold is Min/Max

Feature Type	Colour	Display
metal ion-binding site		<input checked="" type="checkbox"/>
O-phosphorylated L-serine		<input checked="" type="checkbox"/>
O-phosphorylated L-threonine		<input checked="" type="checkbox"/>
O4'-phosphorylated L-tyrosine		<input checked="" type="checkbox"/>
hydrophobic_region		<input checked="" type="checkbox"/>

Optimise Order
 Invert Selection
 Seq sort by Score
 Seq Sort by density

Working with sequence features

Ex 32c,d,e (Sec 2.9.4 P. 80)

- Task
 - Shading features using labels
 - Sorting alignment using features
- Questions
 - What types of features are best displayed with a 'label' colourscheme ?
 - [If feature scores were available] How would you display only the highest or lowest scoring features ?

Protein secondary structure prediction

Section 2.6 onwards
in the Manual

Page 65

File Edit Se



our Calculate

Web Service

MA

Original

Spinach Ferredoxin Structure

Q7XA98_TRIPR/1-152

FER1_MESCR/1-148

FER1_SPIOL/1-147

FER3_RAPSA/1-96

FER1_ARATH/1-148

FER_BRANA/1-96

FER2_ARATH/1-148

	60					70						80												
	M	A	T	Y	K	V	K	L	I	T	P	E	G	P	Q	E	F	D	C	P	D	D	V	Y
	M	A	A	Y	K	V	T	L	V	T	P	E	G	K	Q	E	L	E	C	P	D	D	V	Y
	M	A	A	Y	K	V	T	L	V	T	P	T	G	N	V	E	F	Q	C	P	D	D	V	Y
	-	A	T	Y	K	V	K	F	I	T	P	E	G	E	Q	E	V	E	C	D	D	D	V	Y
	M	A	T	Y	K	V	K	F	I	T	P	E	G	E	L	E	V	E	C	D	D	D	V	Y
	-	A	T	Y	K	V	K	F	I	T	P	E	G	E	Q	E	V	E	C	D	D	D	V	Y
	M	A	T	Y	K	V	K	F	I	T	P	E	G	E	Q	E	V	E	C	E	E	D	V	Y

Secondary Structure



Iron Sulphur Contacts



Alignment

Secondary Structure Prediction

Protein Disorder

Analysis

Conservation

Envision 2

Fetch DB References



Protein Secondary Structure Prediction Sec. 2.6

• Neural network trained on amino acid profiles

- Predicts **Helix**, **shEet**, or **Coil** based on sliding window
 - Also predicts **coiled coils** and **surface accessibilities**

• Server can take

- **Single Sequence**
 - Service find homologs with PSI-Blast
- **Alignment**
 - Service uses MSA to calculate profile for prediction

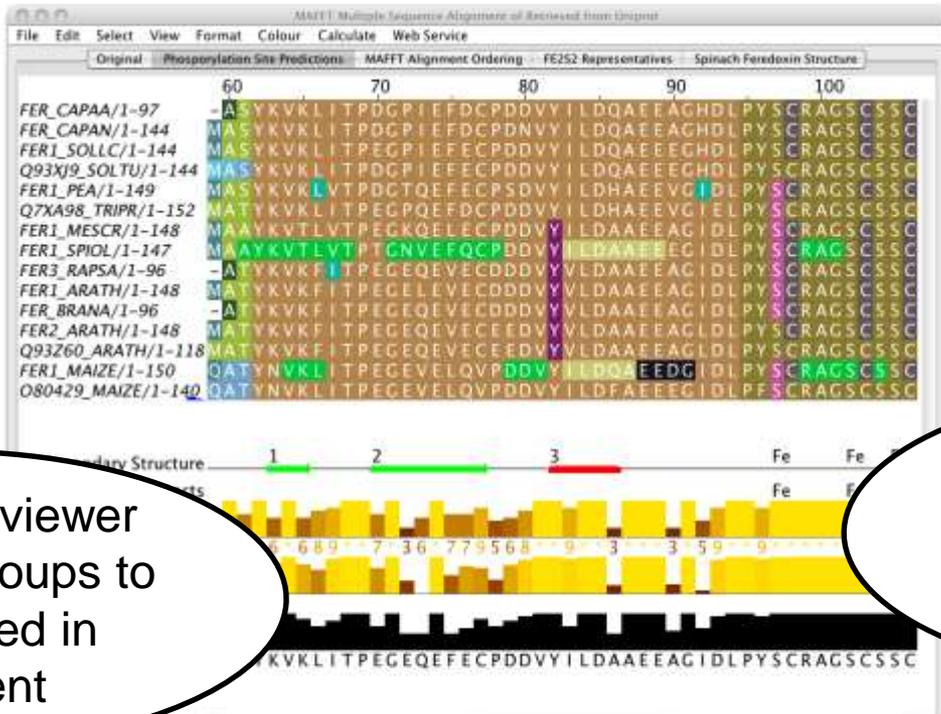
Exercise 26

- Tasks
 - Perform a variety of Jnet predictions
 - Note the effect of hidden regions
 - Learn about sequence associated annotation
- Questions
 - ...

Exercise 26

- Tasks
 - Perform a variety of Jnet predictions
 - Note the effect of hidden regions
 - Learn about sequence associated annotation
- Questions
 - What other data does Jnet provide ?
 - Which is better – a PSI blast prediction or an MSA based prediction ?
 - What happens when you have hidden regions ?

- Session 4
 - Working with structures
 - Viewing 3D structures
 - Mapping data onto structure
 - Disorder prediction
 - Alignment reliability
 - RNA Structure

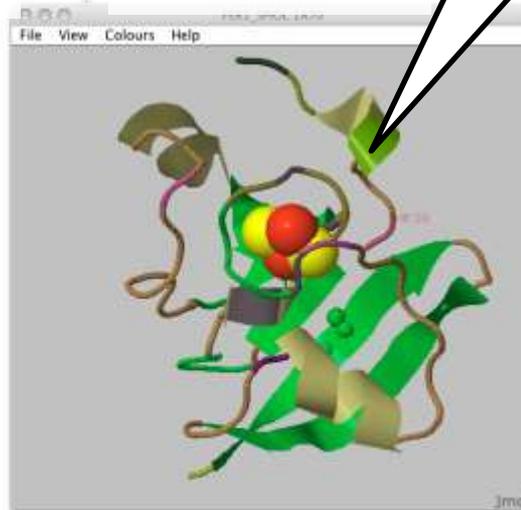
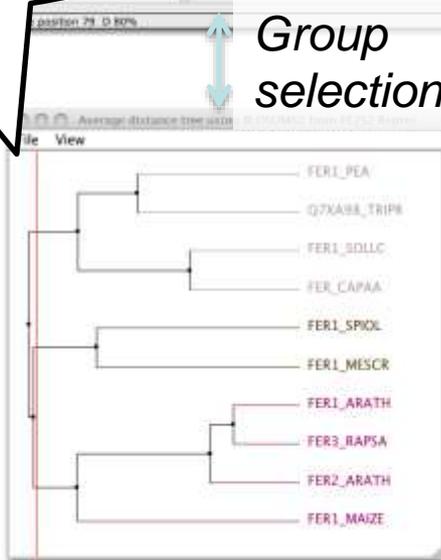


Linked tree viewer allows subgroups to be identified in alignment

Linked Jmol viewer shows one or more structures coloured by alignment

Group selections

Colours and mouseovers



Desktop Structure Visualization

3D structures and 2D RNA diagrams



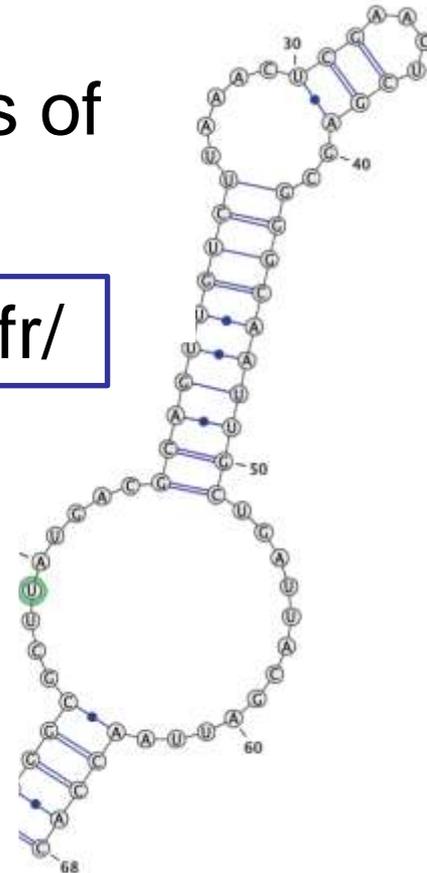
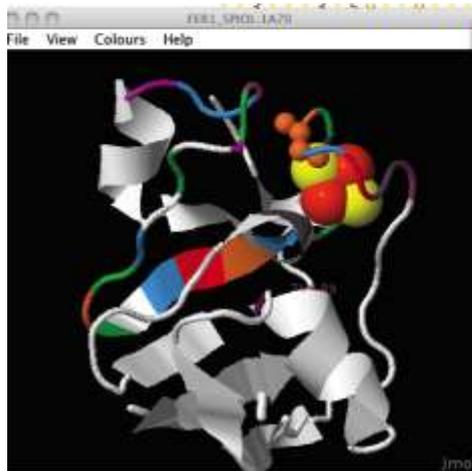
Jmol

<http://jmol.sourceforge.net/>

VARNA

Visual Analysis of
RNA

<http://varna.lri.fr/>



Associating structures with sequences

- Local PDB file
 - Attach PDB file to sequence manually
 - drag and drop to match files to sequences by ID
- Structures in the PDB database
 - Provide PDB id (and chain) for sequence
 - Discover references *via* sequence database



Protein Structures in Jalview

Sec 2.1. Exercise 14

- Task
 - Discover PDB structures for ferredoxin sequence(s)
 - **Note use**
Fetch Database Refs->UNIPROT->Uniprot
 - Save and load structures and manipulate colouring

Protein Structures in Jalview

Sec 2.1. Exercise 14

- Task
 - Discover PDB structures for ferredoxin sequence(s)
 - Save and load structures and manipulate colouring
- Questions
 - How does Jalview match up sequence data to structural data

```
LIVNGGIIAPSFDDP.MDEKAREILQKLFPEHEVVMA.PGRELLL...L...
YIANGGIIAPQFGDPIRDKEAIRVLSDTFPHHSVVG IENAREIVL.A...
LILNNRVFVVPVNGPASVDNDALNVYKTAMPGYEIIIGVKGASGTPWL.TDAL.R.HEVA
LITNKGVI VPPQYGDE.NDALALKQVQEMFPDREIVGV.NTVEVVY...
YVCNGGVVLCAFGDP.NDELAAGIFRRLFPERTVTLV.DARTIFA...G...
YTANGGIVFPLFNDP.MDEKAQEILQKLYPDRKIVGV.PAREILL...I...
L...V...
```

Q8KCB6_CHLTE:1XKN Method: X-ray Chain:A...

File View Colours Jmol Help

Show Chain

- All
- ✓ 1XKN:A
- ✓ 2CMU:A
- ✓ 1VKP:A
- ✓ 1VKP:B
- ✓ 2EWO:A
- 2EWO:B
- 2EWO:C
- 2EWO:D
- 2EWO:E
- 2EWO:F
- 2EWO:G
- 2EWO:H
- 2EWO:I
- 2EWO:J
- 2EWO:K
- 2EWO:L

CYS 366:A

Jmol

many structures can be shown in a single view

Structures can be Superimposed using the visible region of alignment

Superposing Structures using Alignments

Sec 2.1.4 – Exercise 15

- Task
 - Align structures using the ferredoxin alignment

If 'View all N structures' doesn't align structures:

- **Use Jmol->Align menu**
- Experiment with views to control what part of the alignment is used to superimpose the structures

Superposing Structures using Alignments

Sec 2.1.4 – Exercise 15

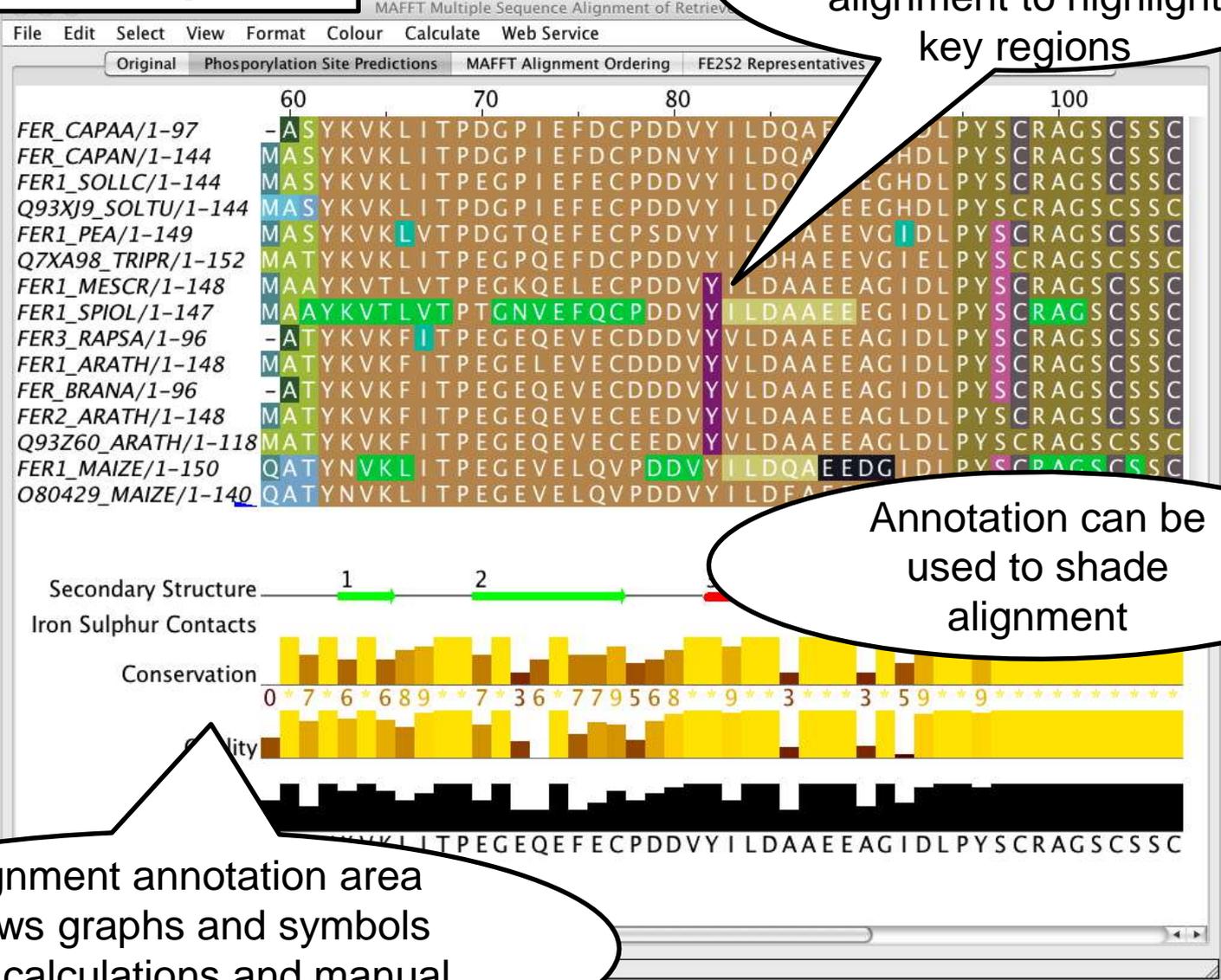
- Task
 - Align structures using the ferredoxin alignment
 - Experiment with views to control what part of the alignment is used to superimpose the structures
- Questions
 - What colourscheme would highlight the conserved parts of the structures ?
 - Which view gave the ‘best’ structure superposition ?
 - How did you decide this ?

Supplementary exercises

- View the PDF from www.jalview.org/training/tutorial-materials/2014/Dundee/Oct
- 3 Short exercises
 - Protein Disorder prediction
 - Calculating/importing alignment quality scores
 - RNA Secondary & Tertiary structure

Just to recap...

Sequence features are overlaid on alignment to highlight key regions



Annotation can be used to shade alignment

Alignment annotation area shows graphs and symbols from calculations and manual curation

Protein Disorder prediction

(Supplementary Exercise)

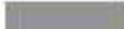
- Complementary problem to secondary structure prediction
 - Recognise structured & unstructured domains
 - Predict holes in density maps (REM450)
 - Detect flexible loops ('HOTLOOPS')
- Programs provided by JABAWS 2 employ
 - Machine learning methods (**DisEMBL**)
 - Similarity to disordered sequences (**RONN**)
 - Empirical amino acid statistics (**IUPred**, **GlobPlot**)

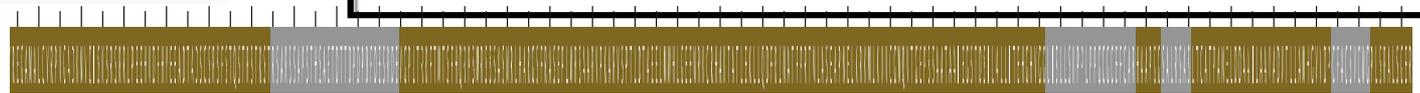
Disorder Predictions from JABAWS

JABAWS
Analysis
Service

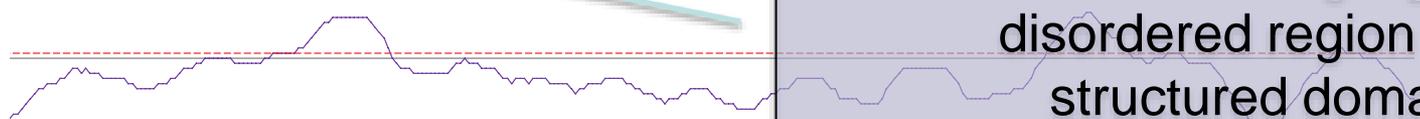
*Disorder
Predictions*

Create **annotation and
features**

<input checked="" type="checkbox"/> DisembiWS	<input checked="" type="checkbox"/> GlobPlotWS	<input checked="" type="checkbox"/> IUPredWS
Feature Type	Colour	Display
Protein Disorder		<input checked="" type="checkbox"/>
COILS		<input type="checkbox"/>
REM465		<input type="checkbox"/>
HOTLOOPS		<input type="checkbox"/>
Globular Domain		<input checked="" type="checkbox"/>



GlobPlotWS (Dydx)



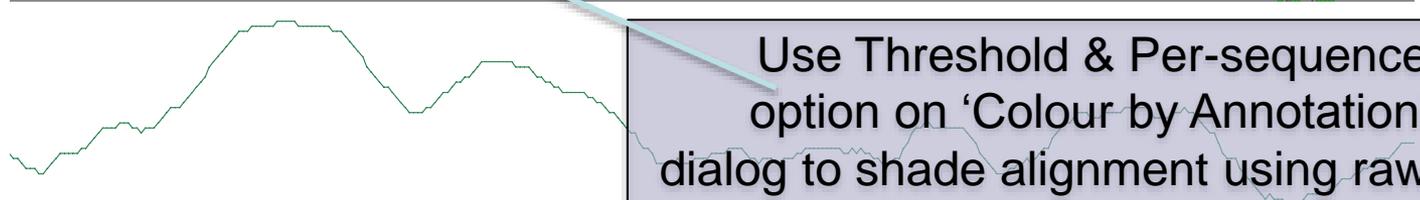
IUPredWS (Short)



IUPredWS (Long)



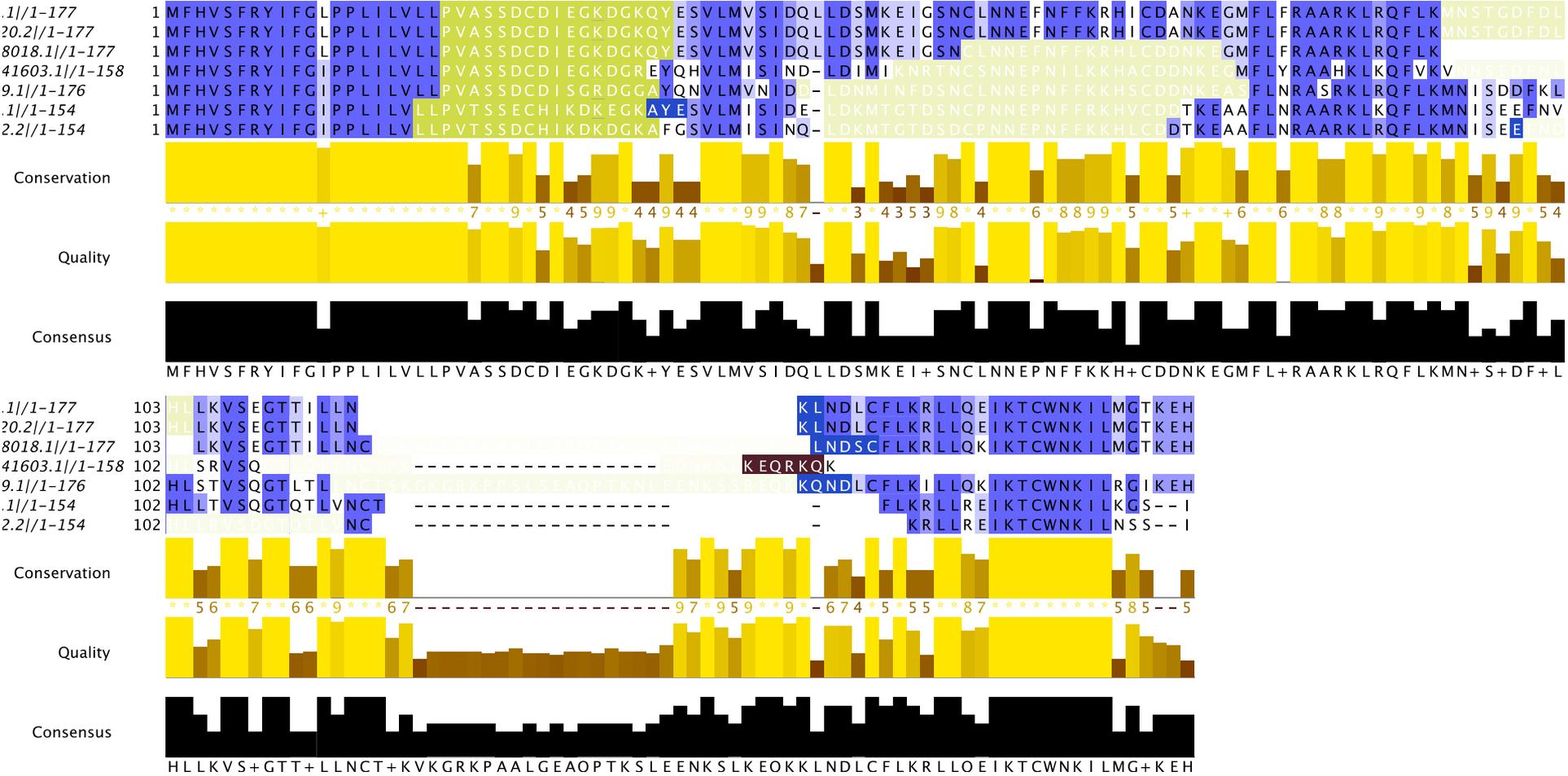
JronnWS (JRonn)



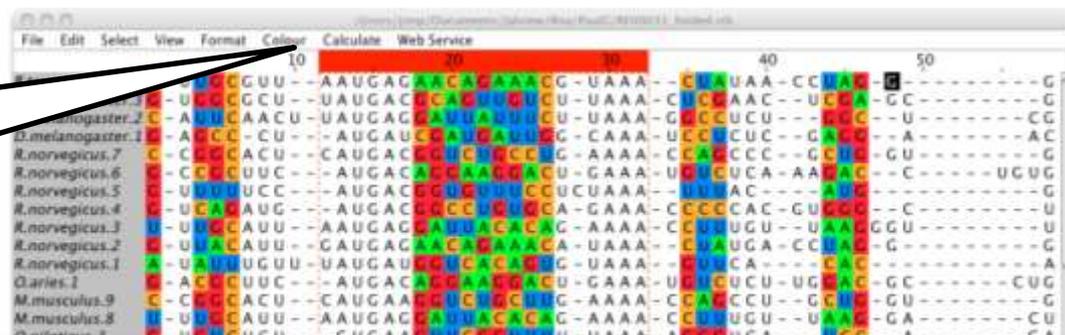
Features highlight
disordered region or
structured domain
predictions

Use Threshold & Per-sequence
option on 'Colour by Annotation'
dialog to shade alignment using raw
scores

Disorder in Interleukin 7



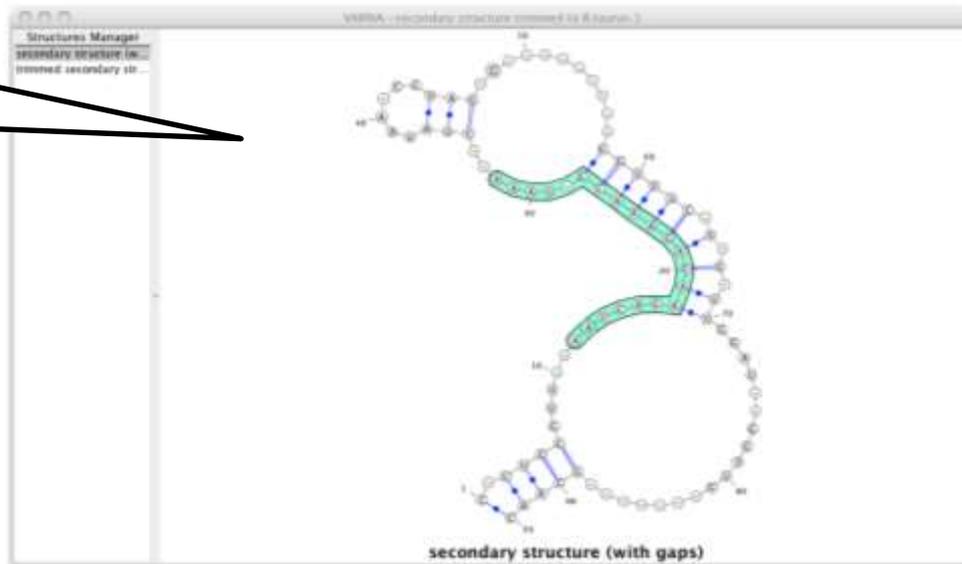
Selections and mouse positions shared between alignment view and VARNA



Try it now:

1. Open VARNA with
'Structure->View Structure->RNA Secondary Structure'
2. Explore difference between trimmed and untrimmed
3. Bonus points – add and link a **Jmol structure view**
Bacillus_amyloliquef.9 corresponds to PDB 3NPB

VARNA has a wide range of 2D RNA plots and supports interactive annotation



VARNA: Interactive drawing and editing of the RNA secondary structure

Kévin Darty, Alain Denise and Yann Ponty

Bioinformatics (2009) **25** 1974-1975

2.8.1 - Interactive Alignment based RNA 2nd-ary Structure Prediction

ViennaRNA

Web Service

Alignment ▶

Secondary Structure Prediction ▶

Protein Disorder ▶

Analysis ▶

Conservation ▶

Fetch DB References ▶

JNet Secondary Structure Prediction

<http://www.compbio.dundee.ac.uk/jabaws>

RNAAliFold Prediction

Change RNAAliFold settings...

Modify settings for the RNAAliFold prediction. Use this to hide or show different results of the RNA calculation, and change RNA folding parameters

```
A - CCUUUGU--UAAGGGU-----UUG
A - -CUAUGA-CCUAG-G-----GGU
A - -GUUCA----CAC-----AGC
A - UGUCUCU-UGGAC-GC-----CUGGU
A - CCAGCCU--GCUG-GU-----GGG
A - CCUUUGU--UAAG-GA-----CUUG
A - AGGGUCA---UCC--A-----GAAA
```

2.8.1 - Interactive Alignment based RNA 2nd-ary Structure Prediction

ViennaRNA

```
D.melanogaster.5/1-68 G - UGGCGCU
D.melanogaster.2/1-63 C - AUUCAAC
D.melanogaster.1/1-65 G - AGCC - CU
R.norvegicus.7/1-66 C - CGGCACU
R.norvegicus.6/1-67 G - CCGCUUC
R.norvegicus.5/1-62 G - UUUUUC
R.norvegicus.4/1-61 G - UCAGAUG
```

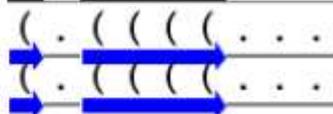
```
Consensus G UUC
           ACGG
           CGAUG
G - UUUCAUU
```

RNAalifold Consensus B - H B K S W Y Y

Contact Probabilities



Centroid Structure



MFE Structure



StrucConsensus

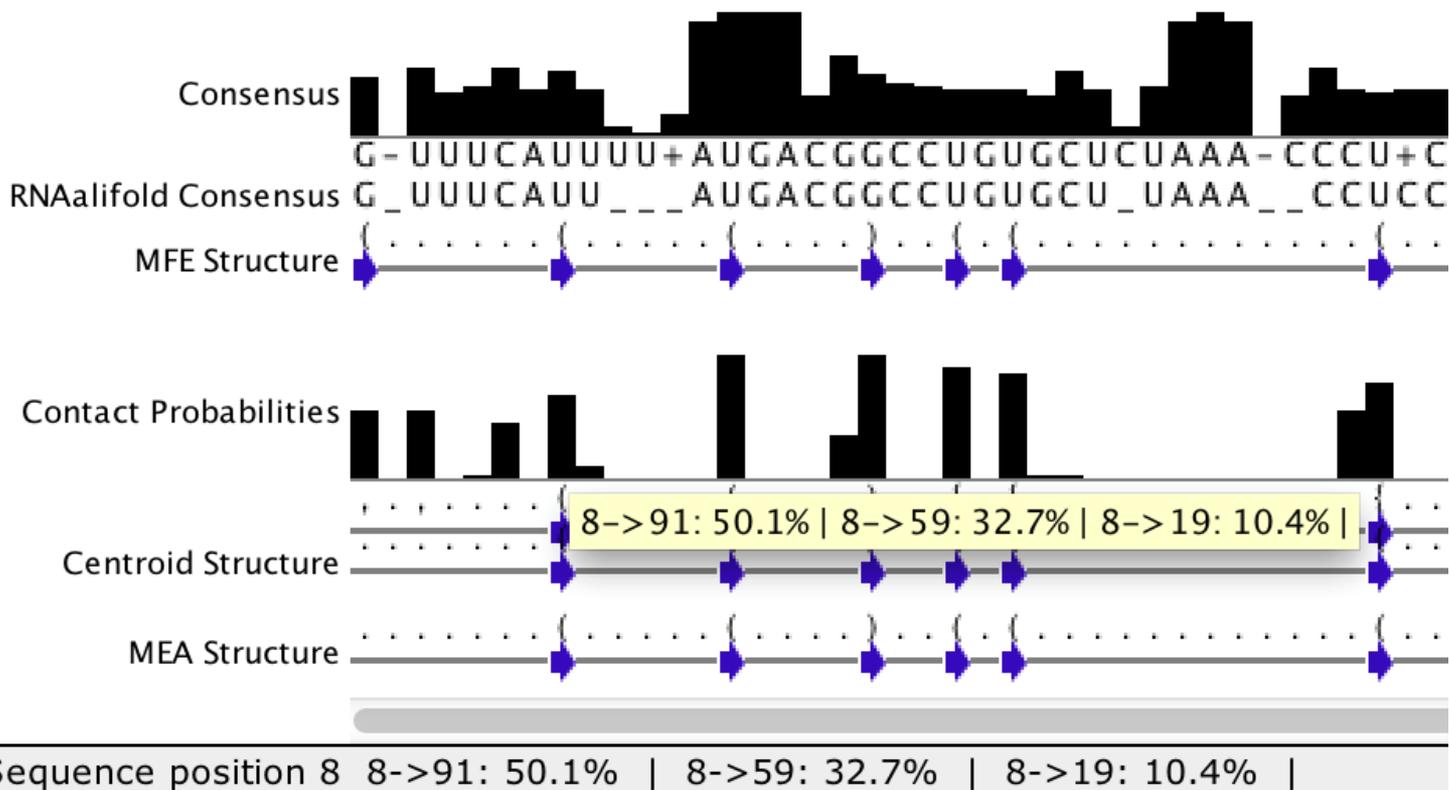
```
GC UACCUAGC
CG ACUAGCCG
UA ACUGCAUA
CU ACUGCAUA
CU ACUGCAUA
(- ( ( ( ( - - -
```

- Can be enabled for any view
- Updated if alignment changes
- settings & results saved in Jalview project

Implemented by our 2013 Summer student

Tooltips show alternative base pairs

R.norvegicus.2/1-64 G - UUACA UU - - GAUGAGAA CAGAAACA - UAAA - - CUAUG
R.norvegicus.1/1-61 A - UAUUUGUU - UAUGAUGGUCACAGUG - UAAA - - GUUCA
O.aries.1/1-68 G - ACGCUUC - - - AUGACAGGAAGGACU - GAAA - UGUCUC



9.00-9.15am.

Overview of the day

9.15am - 10.30am.

Session 1. Introduction to Jalview

- starting the application, importing alignments, basic editing and creating figures.

10.30-11am.

Coffee

11am - 12.30pm.

Session 2: Alignment & alignment analysis

- Creating sequence alignments, importing and calculating trees, tree based alignment analysis

12.30pm to 1.30pm.

Lunch

1.30pm – 3.00pm.

Session 3: Annotating sequences & alignments

- Creating and viewing sequence annotation
- Protein Secondary structure prediction

3.00pm – 3.30pm

Coffee (Late! Sorry !)

3.30pm – 4.30pm.

Session 4: Working with molecular structures

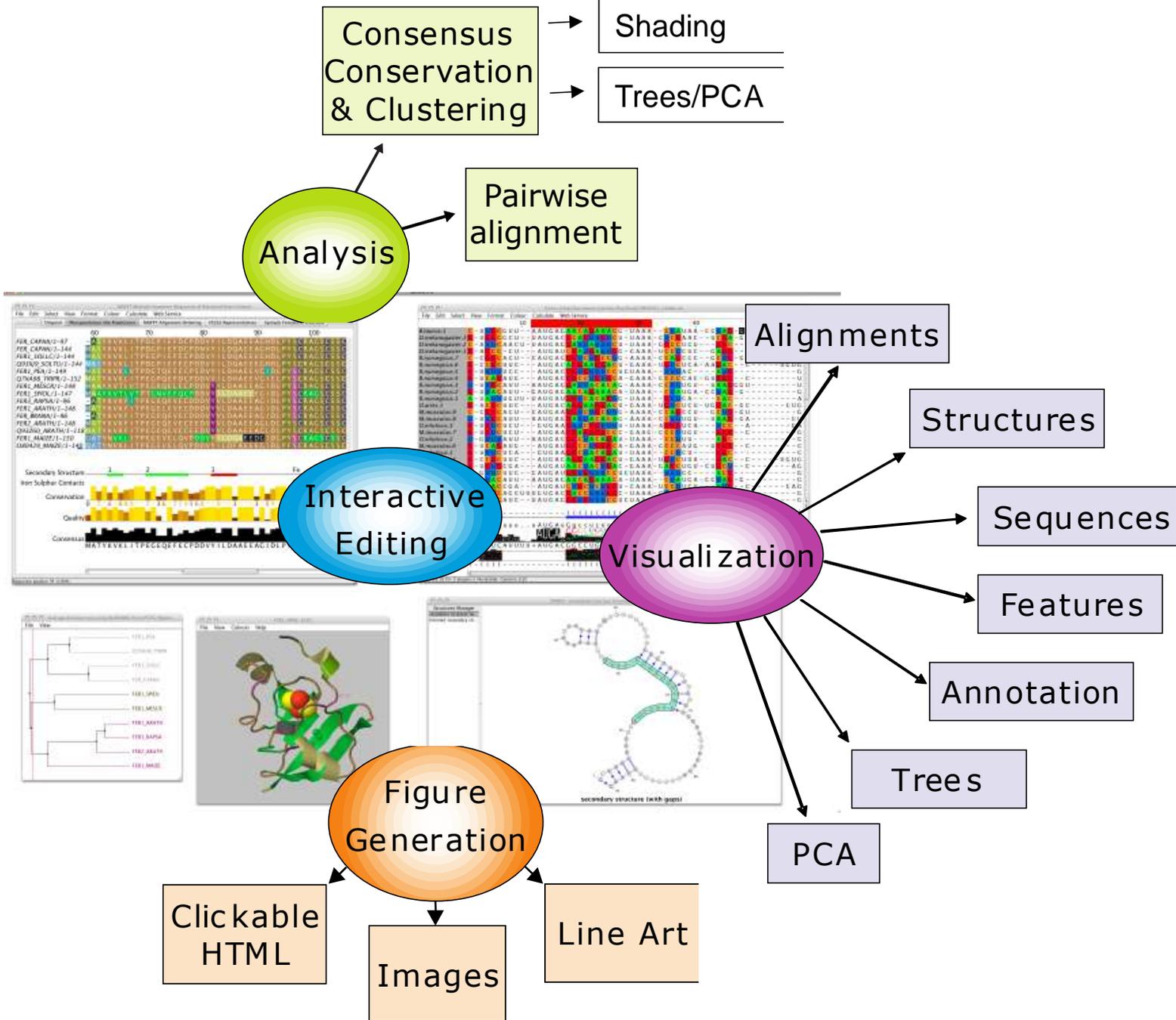
- Viewing 3D Structures, superimpositions, mapping disorder and alignment quality
- Viewing RNA Secondary Structure

4.30pm – 4.45pm.

Wrapup – what we didn't cover today

~5pm

.. And then to Duke's Corner!



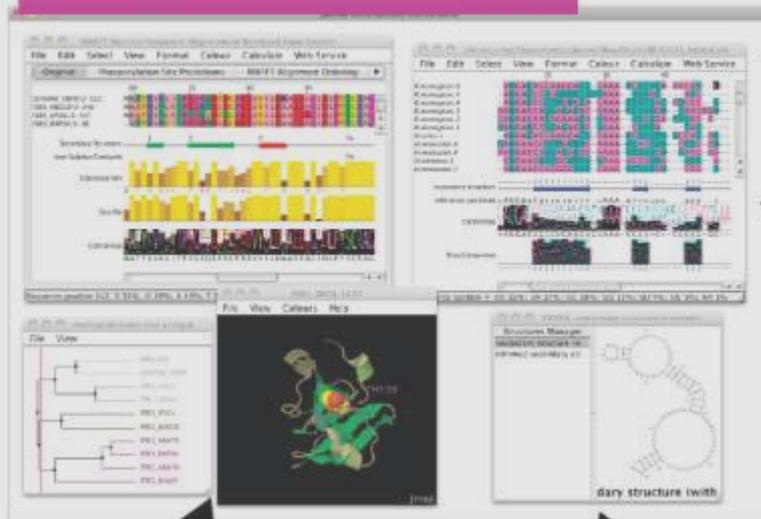
Jalview Flavours

Multi-windowed UI
Visualization & Analysis

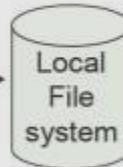
Common Data & Analysis
Editing, messaging and
File Input/Output

Lightweight UI
Integrate with web sites

The Jalview Desktop



Figures
HTML
EPS
PNG



import
from web

Analysis Services

Protein 2ndary structure



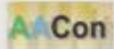
Alignment Analysis



Protein Disorder

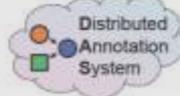
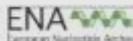
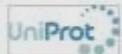


Multiple alignment



GLOBPLOT 2

Biological Data Services



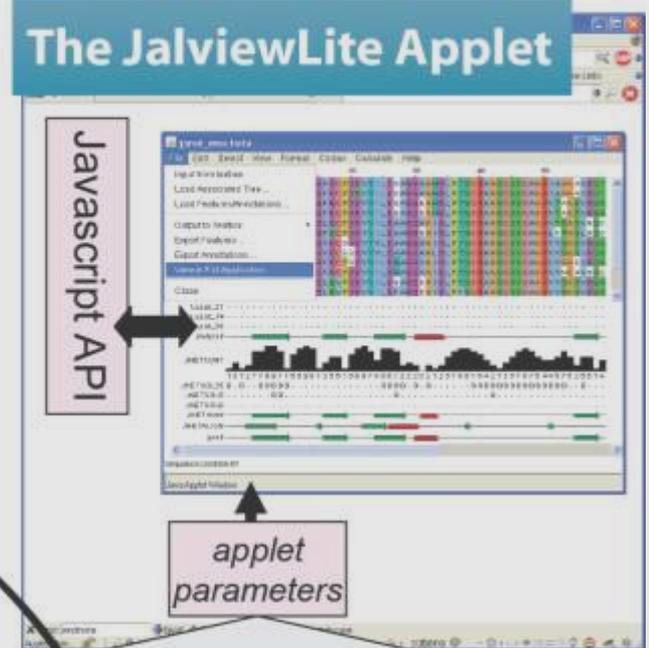
The JalviewLite Applet

Javascript API

applet
parameters

Alignment
And
Annotation

Bioinformatics
Web Server



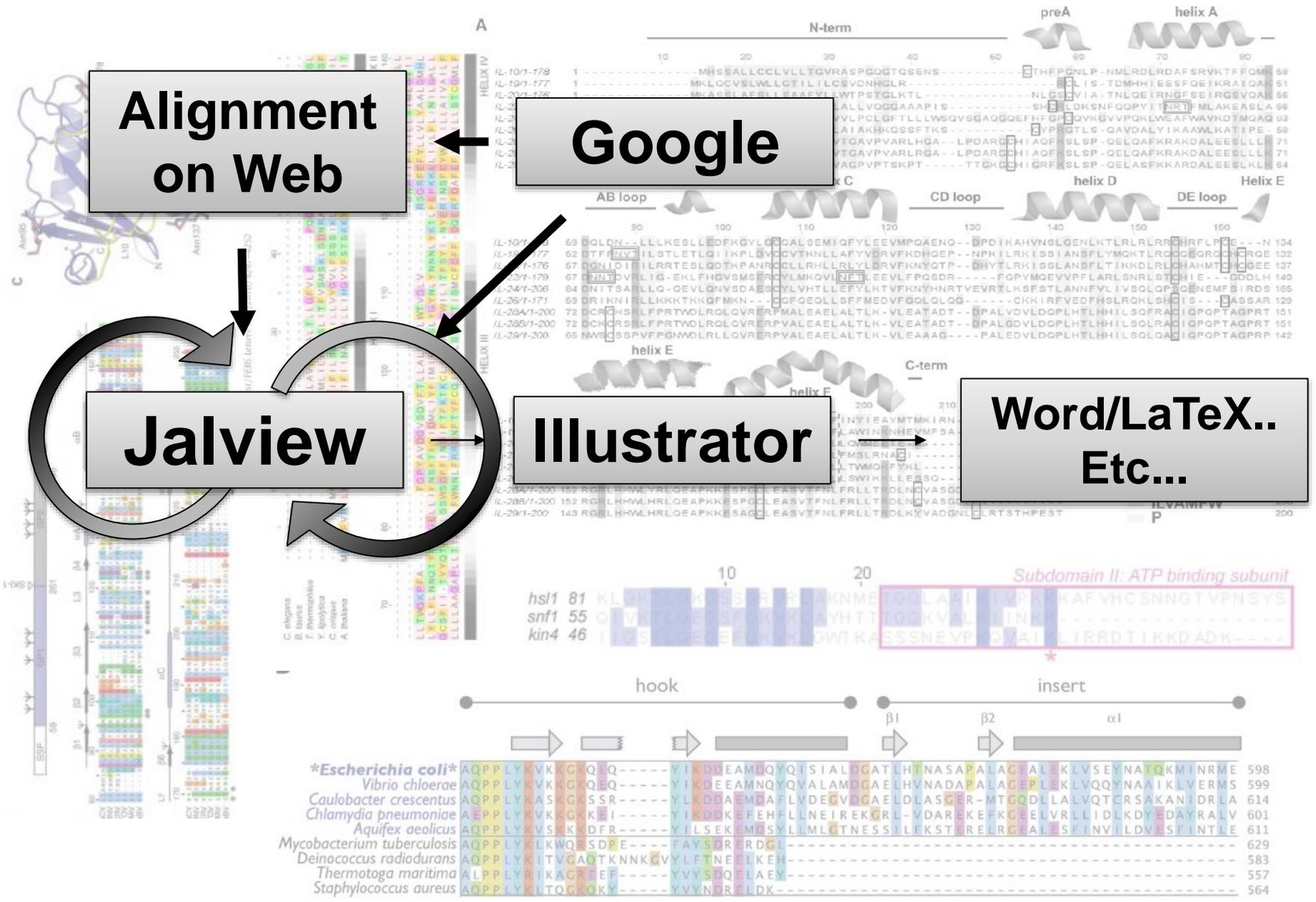
Alignment on Web

Google

Jalview

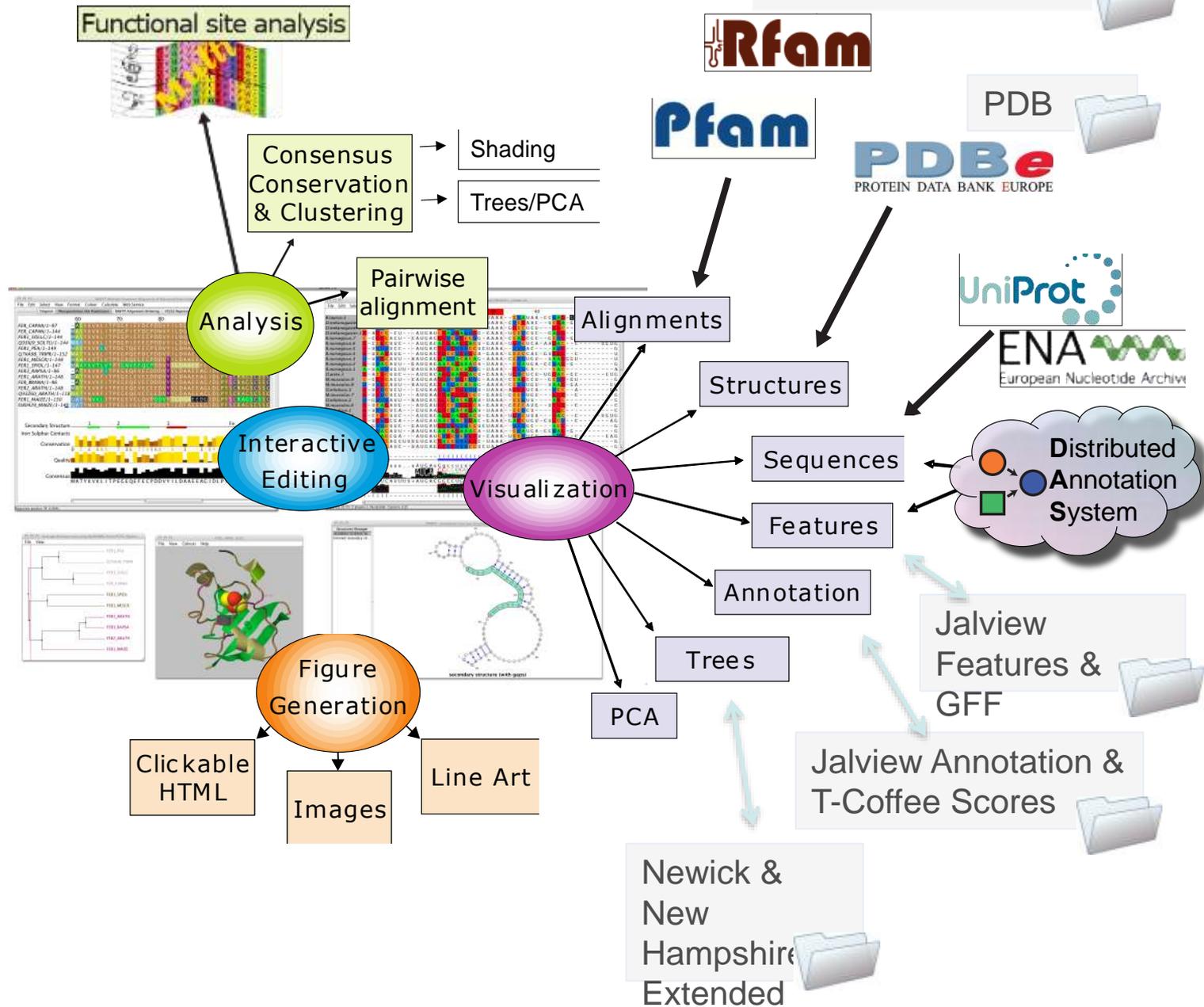
Illustrator

Word/LaTeX.. Etc...



The Jalview Desktop

Clustal Fasta Pile-Up
BLC Stockholm PIR



NEW FOR
2014

ViennaRNA

Ronny Lorenz et al. Algorithms for Molecular Biology, 2011 doi:10.1186/1748-7188-6-26

JPred3

Chris Cole, Jon Barber and Geoff Barton
NAR Web Server Issue 2008

doi:10.1093/nar/gkn238

MSAprobs: multiple alignment with pair HMMs

Yongchao Liu, Bertil Schmidt, and Douglas L. Maskell *Bioinformatics* 2010 26 1958 -1964

GLProbs – adaptive sequence alignment

Yongtao Ye et al. Proc. ACM BCB, 2013 pp.152-160

<http://sourceforge.net/projects/glprobs/>

Analysis

Interactive

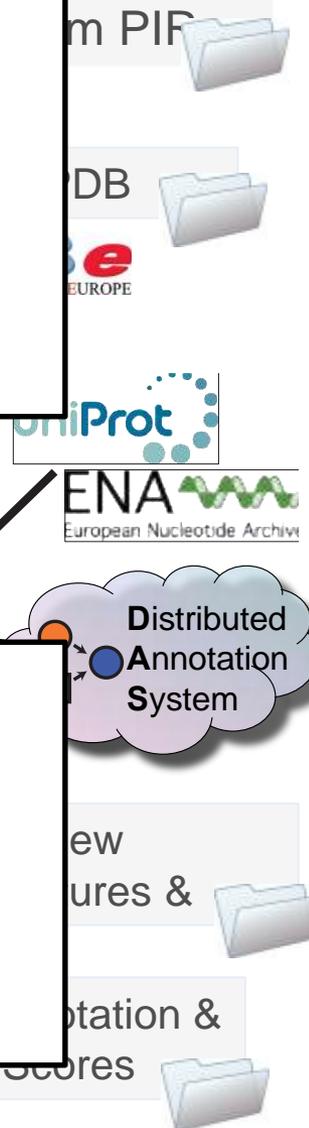
Alignments

Structures

Sequences

Distributed Annotation System

Newick & New Hampshire Extended



DNA and Protein in Jalview

- Discussed in Section 2.10 of manual
- From DNA to Protein
 - Calculations => Translate cDNA
 - View protein annotation on exons using EMBL records
- From protein to DNA
 - Recover DNA for proteins using EMBL cross references

Things I haven't talked about ...

Currently available in v 2.8.1

- Internationalisation (Spanish, so far)
- View flanking regions (Proteomics)
- More score models for PCA/Trees
- View 'representative structures'
- Select columns by feature..

Select column by feature

ment of Retrieved from Uni

Calculate Web Service

tions MAFFT Align

80 90

DDVY I LDHAAEEVGI EL PY SC
DDVY I LDAAEEAGIDL PY SC
DDVY I LDAAEEEGIDL PY SC
DDVY V LDAAEEAGIDL PY SC
DDVY V LDAAEEAGIDL PY SC
DDVY V LDAAEEAGIDL PY SC
EDVY V LDAAEEAGLDL PY SC
EDVY V LDAAEEAGLDL PY SC
DDVY I LDDAEEEDGIDL PY SC
DDVY I LDFAEEEGIDL PY SC

3

6 8 9 3 3 5 9 9

Sequence Feature Settings

Feature Settings DAS Settings

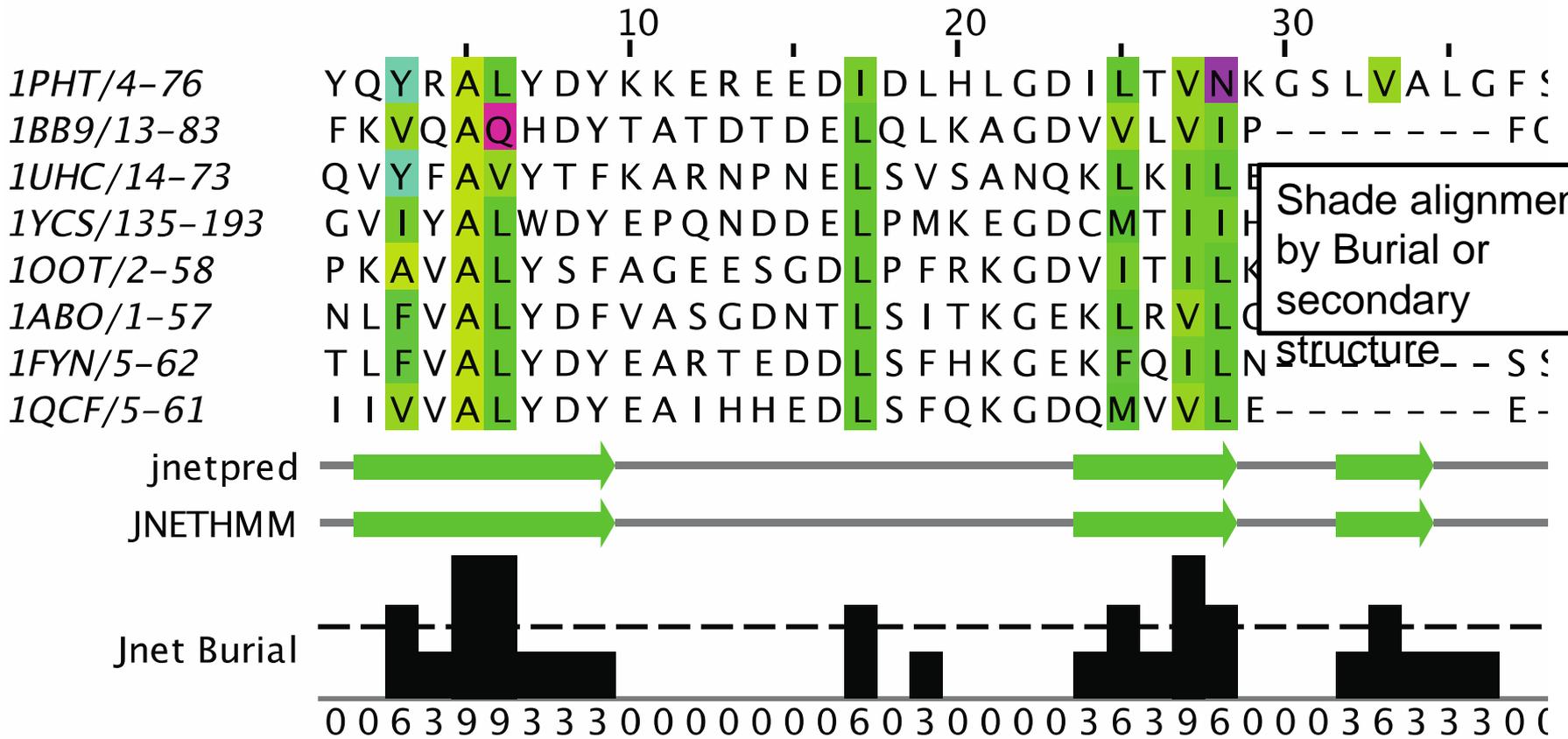
uniprot netphos
 Ia70

Feature Type	Colour	Display
RESNUM		<input type="checkbox"/>
MOD_RES		<input checked="" type="checkbox"/>
VARIANT		<input checked="" type="checkbox"/>
METAL		<input checked="" type="checkbox"/>
PHOSPHORYLATION (S)		<input checked="" type="checkbox"/>
PHOSPHORYLATION (T)		<input checked="" type="checkbox"/>
PHOSPHORYLATION (Y)		<input checked="" type="checkbox"/>
CONFLICT		<input type="checkbox"/>
TURN		<input type="checkbox"/>
HELIX		<input type="checkbox"/>
STRAND		<input type="checkbox"/>

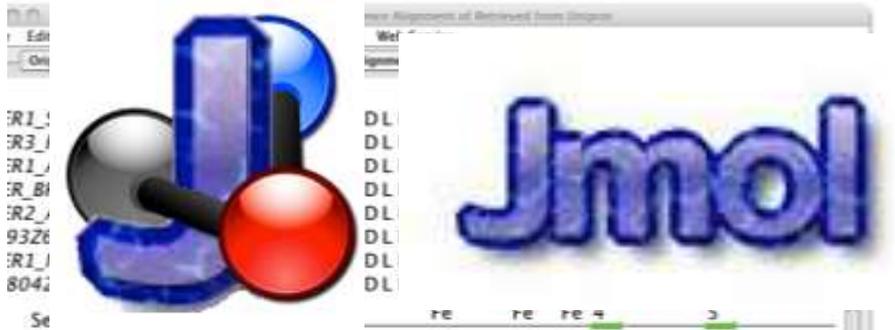
Sort by Score
Sort by Density
Graduated Colour
Select columns containing
Select columns that do not contain

Invert Selection

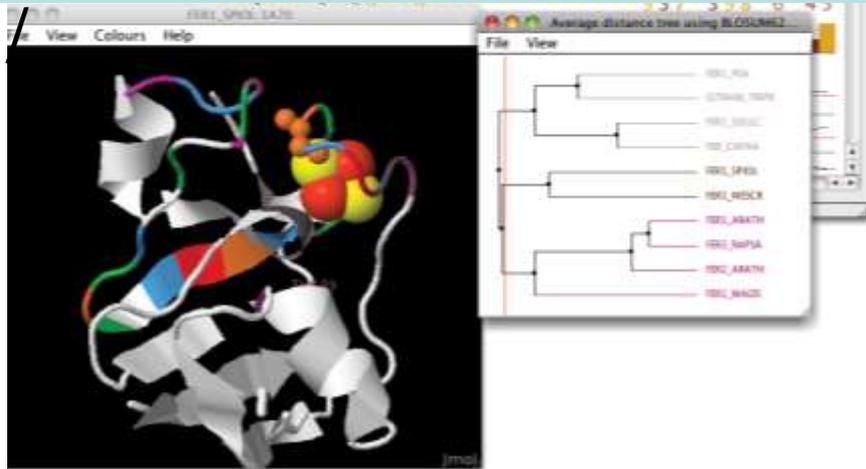
2.8.2 alpha - New look Jpred results



Secondary structure from 3D data



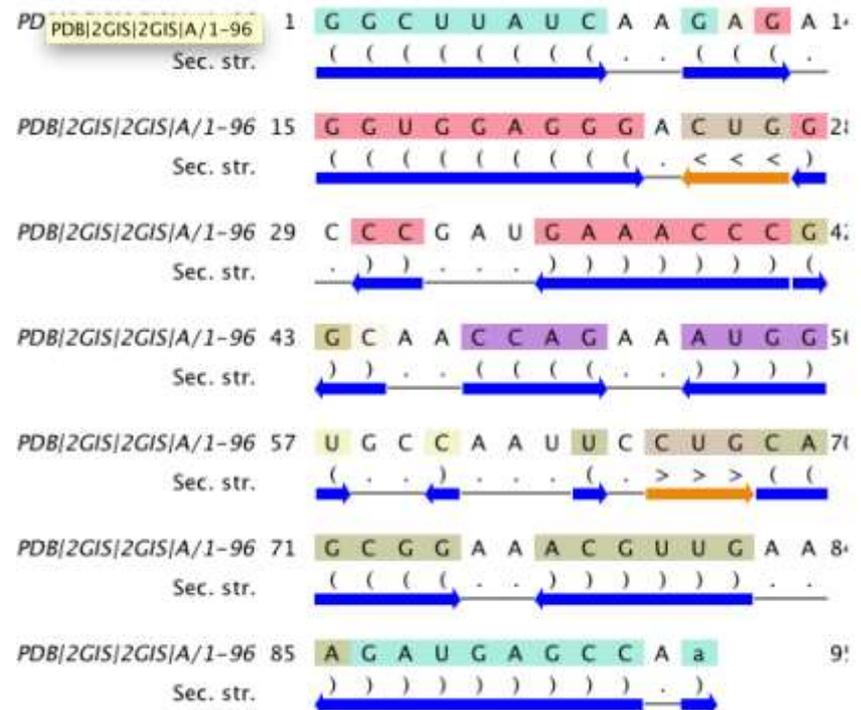
<http://jmol.sourceforge.net>



- Jmol includes a Java port of **DSSP**
 - Courtesy of the Vriend Lab
- Jalview 2.8.2 extracts secondary structure from 3D data

RNAView, pyRNA

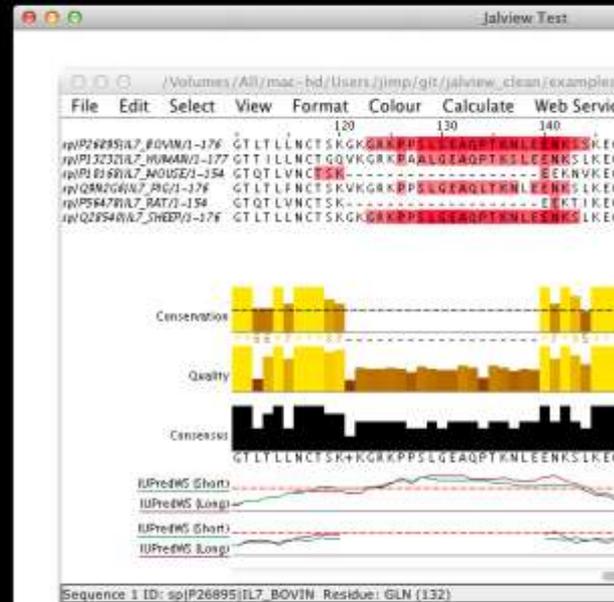
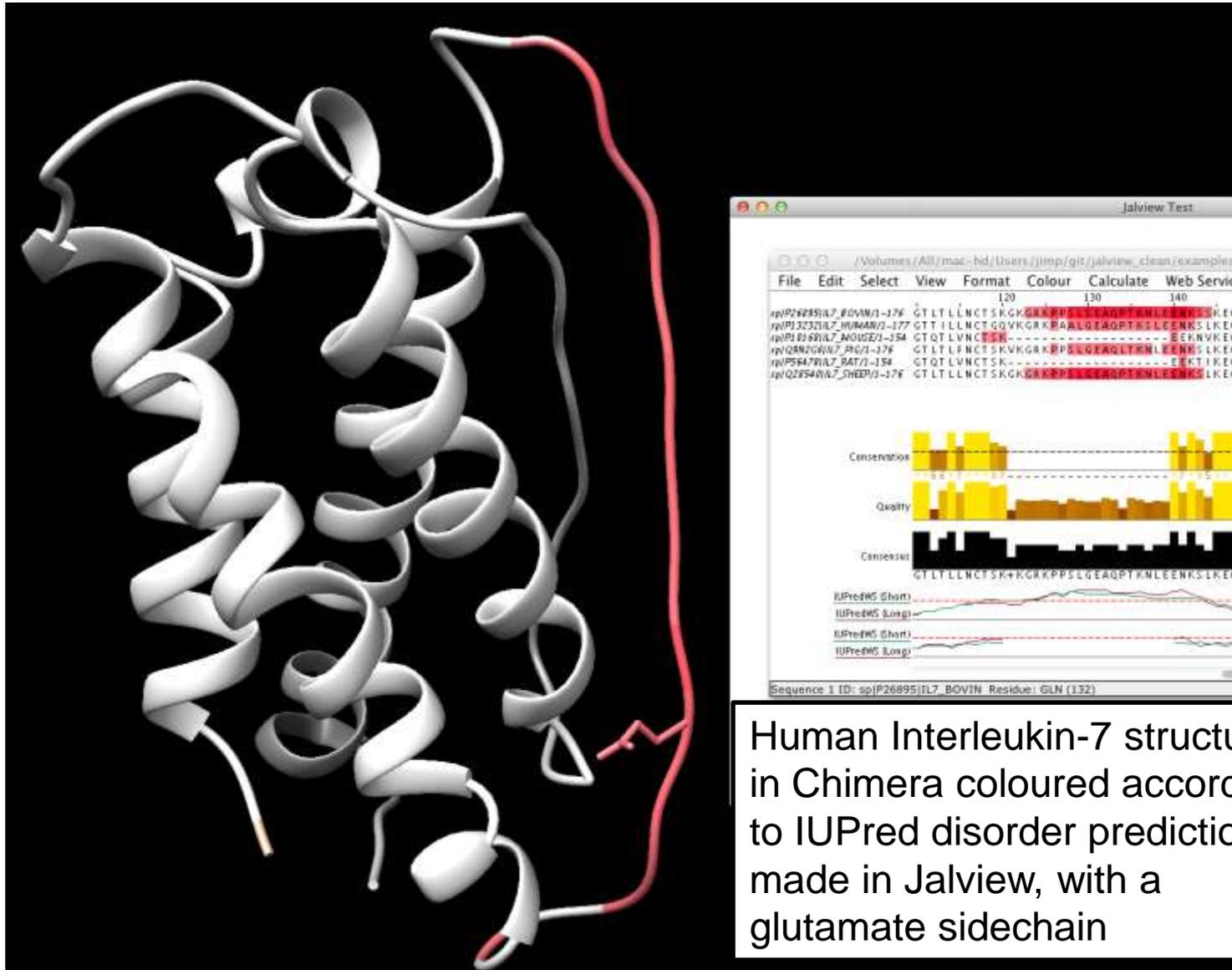
- Fabrice Jossinet's pyRNA server includes RNAView*
 - Identify and characterise base pair interactions in 3D structure
- Used by Jalview to obtain secondary structure for RNA 3D data



* RNAView will shortly be replaced by **DSSR** (Xiang-Jun Lu)

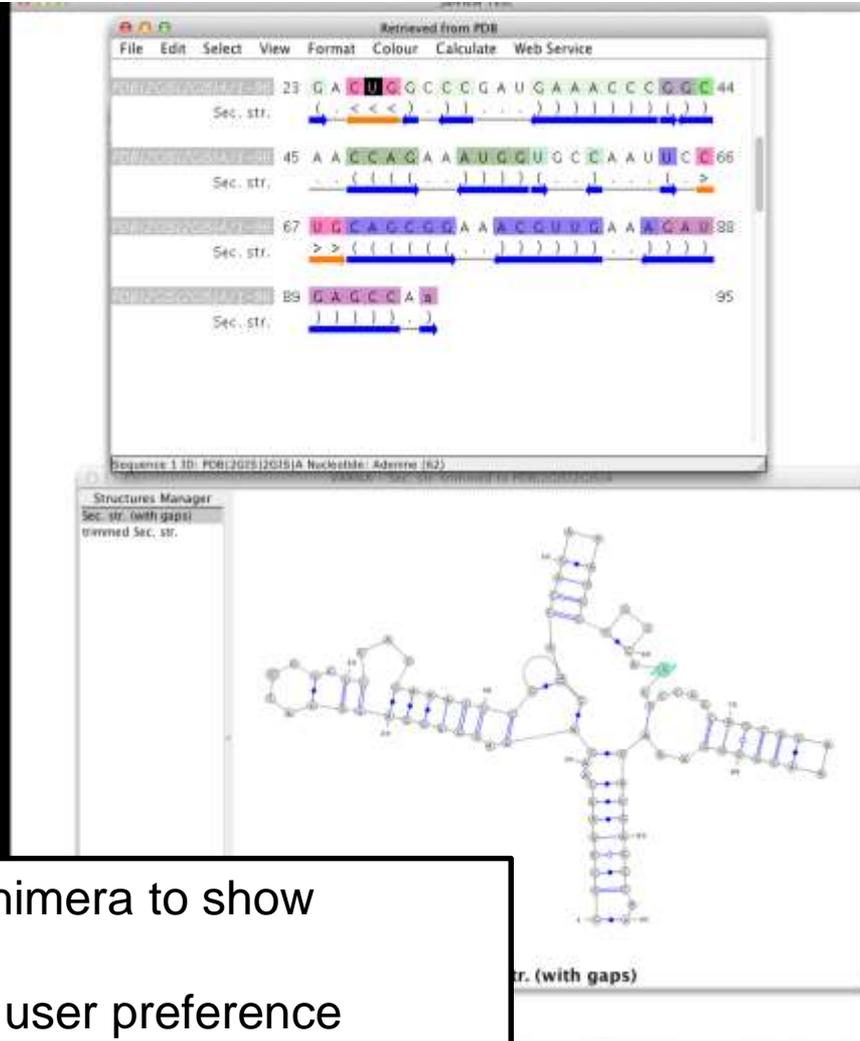
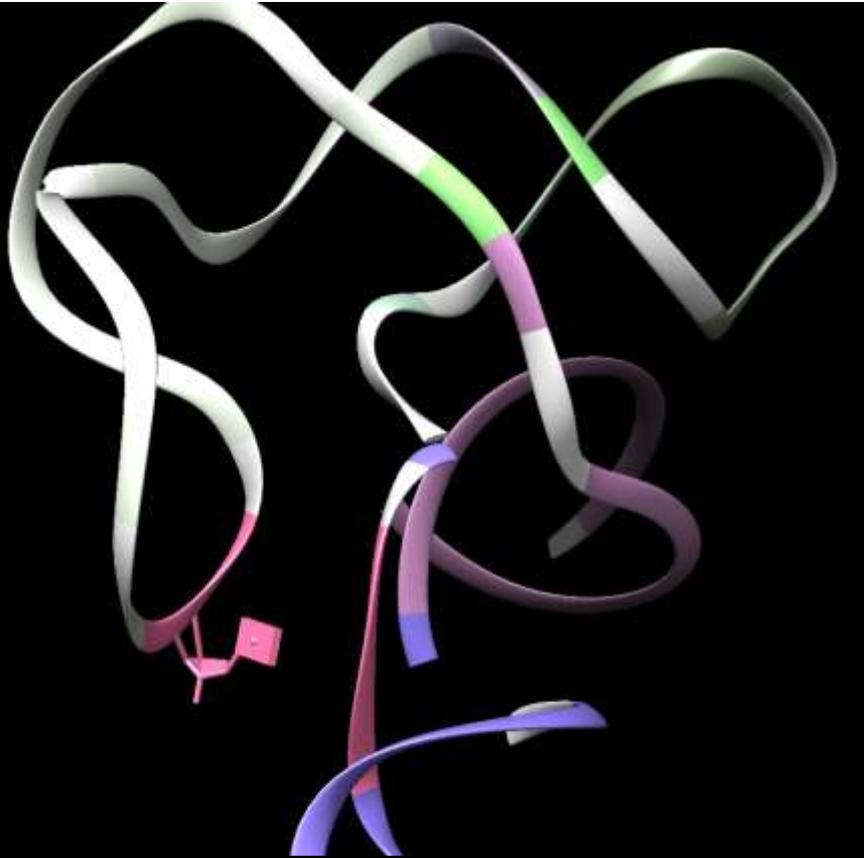
<http://2dnp.org/index.php>

Jalview and Chimera



Human Interleukin-7 structure in Chimera coloured according to IUPred disorder prediction made in Jalview, with a glutamate sidechain

Jalview + VARNA + Chimera



Jalview Desktop uses UCSF Chimera to show structures:

- Optional - Enabled as a user preference
- Structures coloured & superposed like with Jmol
- Positional highlighting from Jalview->Chimera



The Jalview developers
Michele Clamp
Harvard & MIT.



James Cuff
Harvard & MIT



Steve Searle
Sanger, UK



Andrew Waterhouse
Basel, Switzerland.

RNA Features

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Yann Ponty (VARNA)
École Polytechnique,



T-COFFEE Scores
Paolo di Tomasso
Notredame Group, CRG, Spain.

Geoff Barton

- David Martin (**Teaching**)
- Sasha Sherstnev (**JABAWS**)
- Peter Troshin (**JABAWS**)
- Barry Strachan (**logo**)
- Tom Walsh (**Apache**)
- Ryan Maclaughlan (**CSS**)
- Andrew Millar (**Drupal**)
- All the Jalview users, and

...

JALVIEW



supported by

