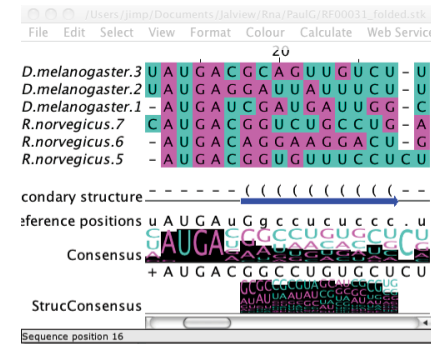
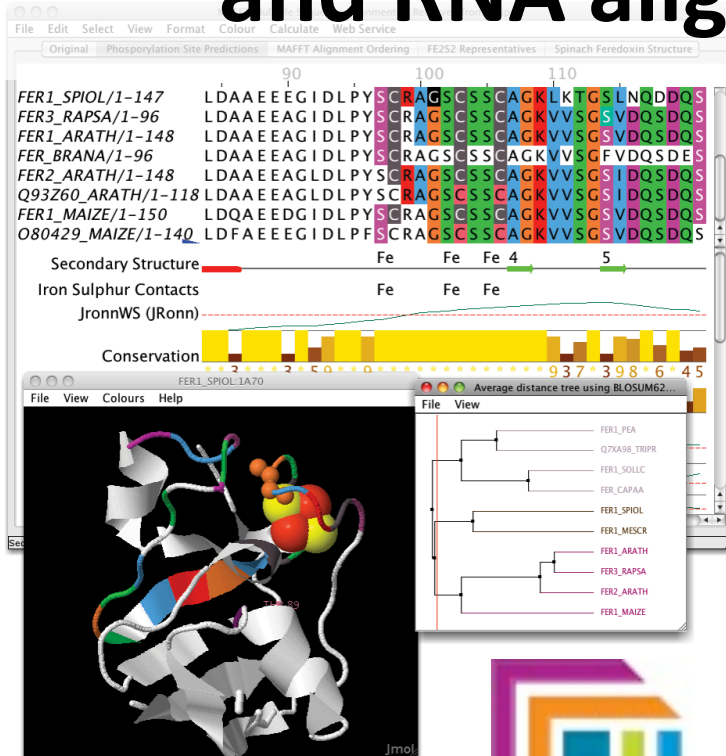


Creation, curation and analysis of Protein and RNA alignments with Jalview



Jalview
www.jalview.org

Jim Procter, Jalview Coordinator

j.procter@dundee.ac.uk

Scottish Phylogeny Discussion Group

James Hutton Institute 18th February 2013



The Barton Group
School of Life Sciences, University of Dundee, Dow St, Dundee DD1 5EH, Scotland, UK

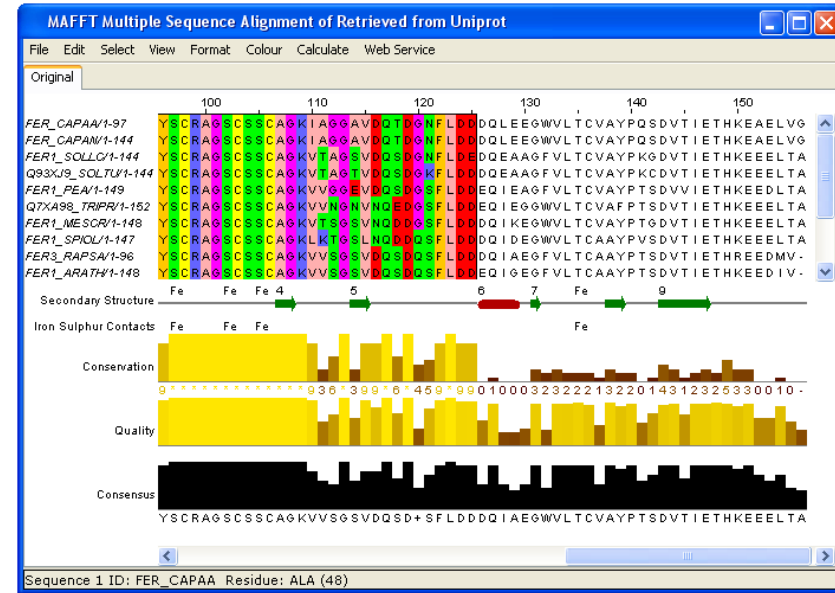


BBSRC
bioscience for the future



What is Jalview ?

- A java alignment viewer
*j*ava *al*ignment *view*er
.. but not just for viewing..
- Java ?
 - Platform independence
 - Standalone or web based tool

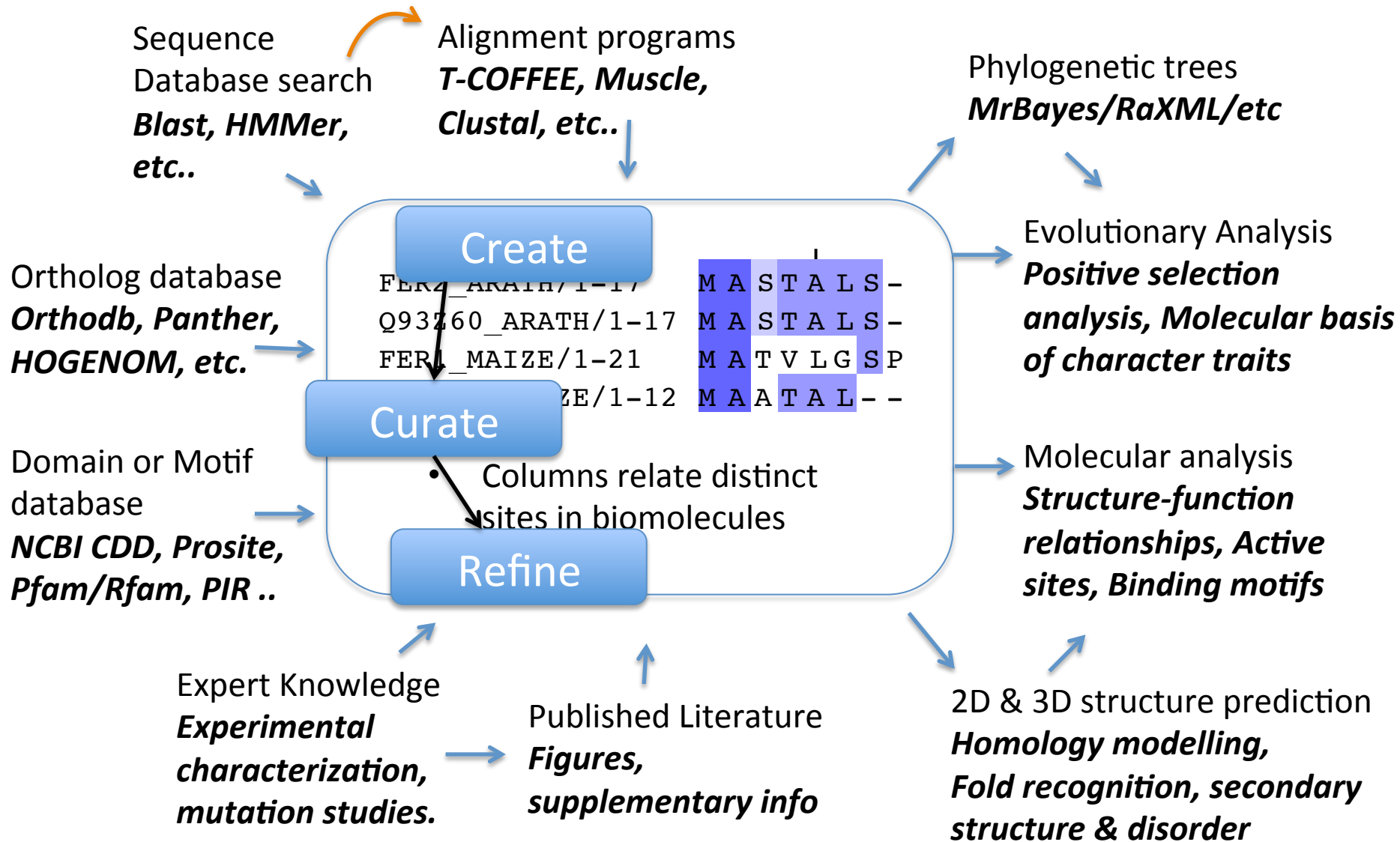


- Open source since '98
 - Coordinated in Dundee
 - Core development funded by ...



The Barton Group
School of Life Sciences, University of Dundee, Dow St, Dundee DD1 5EH, Scotland, UK



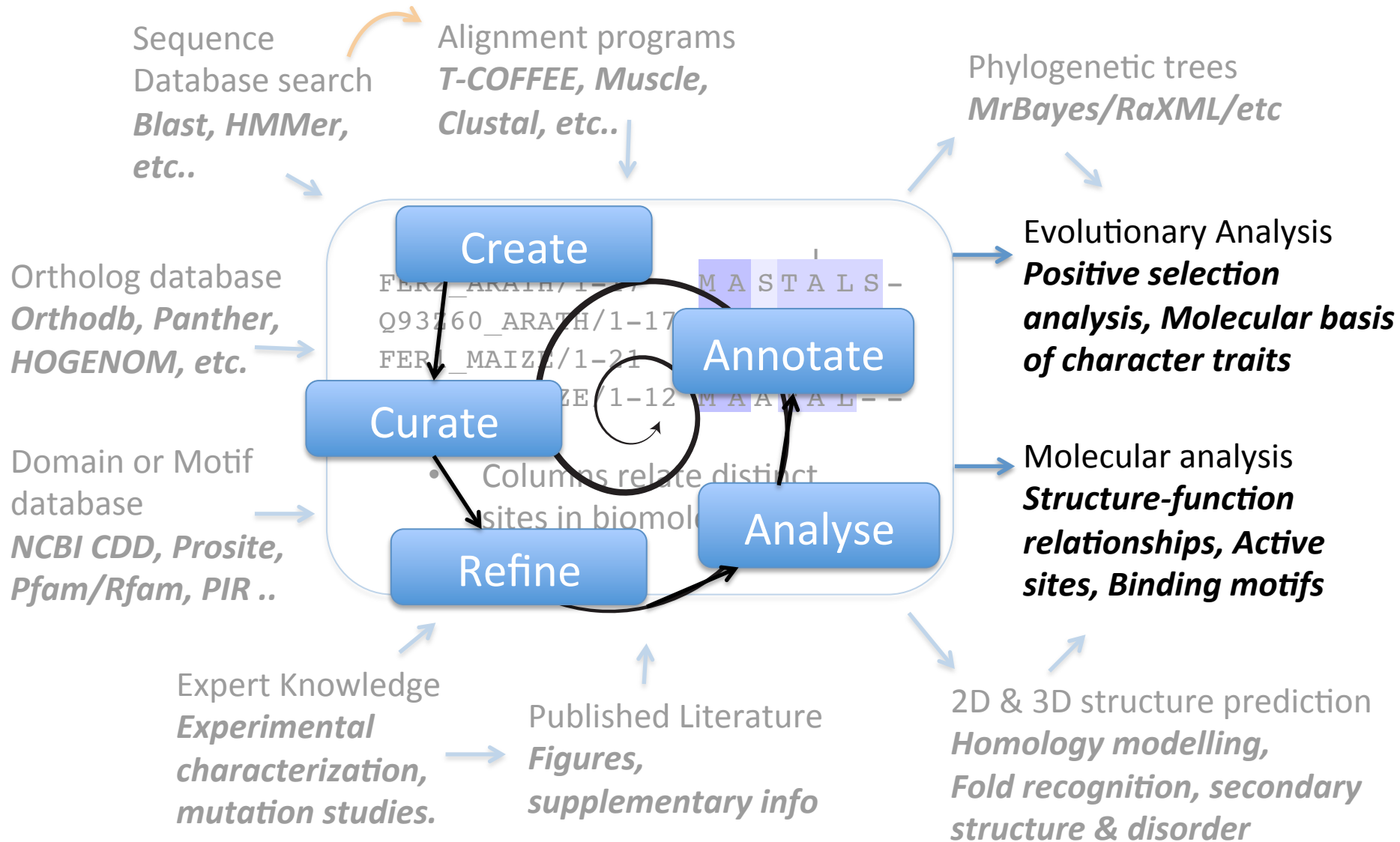


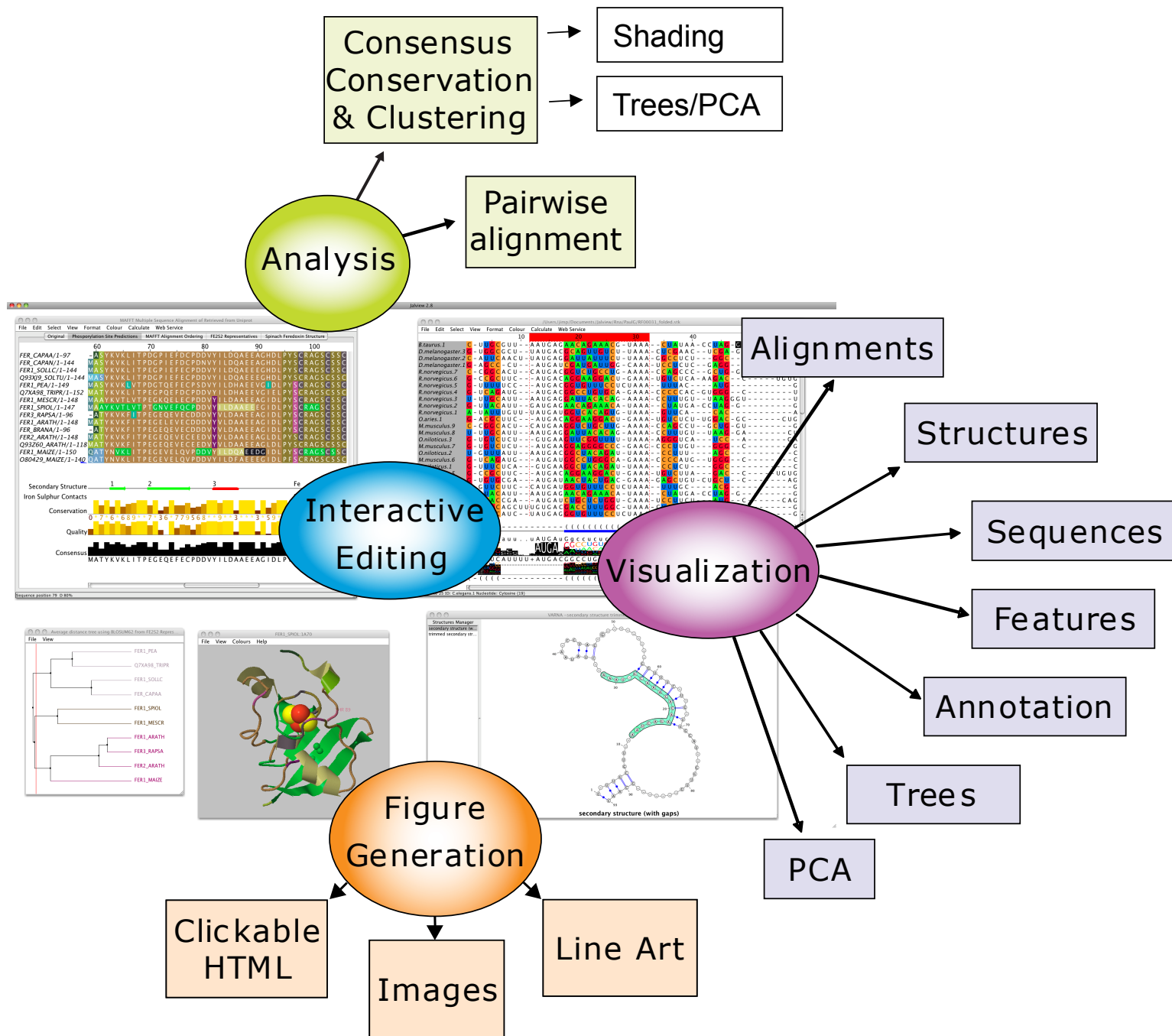
Curating Alignments

- Alignments sometimes need manual curation
- Correct alignments conserve common properties
- Shading can highlight differences

FER_CAPAA/28-82	AEEAGHDLPYSCRAGSCSSCAGKIAGGAVDQTDGNFLDDQLEEGWVLTCAVAYPQ
FER_CAPAN/75-129	AEEAGHDLPYSCRAGSCSSCAGKIAGGAVDQTDGNFLDDQLEEGWVLTCAVAYPQ
FER1_LYCES/75-129	AEEEGHDLPYSCRAGSCSSCAGKVTAGSVDSQDGNFLDEQEAAGFVLTCVAYPK
Q93XJ9_SOLTU/75-129	AEEEGHDLPYSCRAGSCSSCAGKVTAGTVDSQDGKFLDDQEAAGFVLTCVAYPK
FER1_PEA/80-134	AEEVGIDLPYSCRAGSCSSCAGKVVGGEVDQSDGSFLDDEQIEAGFVLTCVAYPT
Q7XA98_TRIPR/83-137	AEEVGIELPYSCRAGSCSSCAGKVVGNGVNGEDGSFLDDEQIEGGWVLTCAVAFPT
FER1_MESCR/79-133	AEEAGIDLPYSCRAGSCSSCAGKVTSGSVNQDDGSFLDDQIEKGWVLTCAVAYPT
FER1_SPIOL/78-132	AEEEGIDLPYSCRAGSCSSCAGKLKTGSLNQDDQSFLDDQIDEGWVLTCAAYPV
FER3_RAPSA/28-82	AEEAGIDLPYSCRAGSCSSCAGKVVSQSVDSQSDQSFLDDQIAEGFVLTCAYPT
FER_ARATH/80-134	AEEAGIDLPYSCRAGSCSSCAGKVVSQSVDSQSDQSFLDDEQIEGEGFVLTCAYPT
FER_BRANA/28-82	AEEAGIDLPYSCRAGSCSSCAGKVVSQFVDQSDQSFLDDQIAEGFVLTCAYPT
FER2_ARATH/80-134	AEEAGLDLPYSCRAGSCSSCAGKVVSQSIDQSDQSFLDDEQMSSEGYVLTCVAYPT
FER1_MAIZE/80-134	AEEDGIDLPYSCRAGSCSSCAGKVVSQSVDSQSDQSYLDDGQIADGWVLTCHAYPT
O80429_MAIZE/72-126	AEEEGIDLPFSCRAGSCSSCAGKVVSQSVDSQSDQSF LNDNQVADGWVLTCAAYPT

Alignments are central ...





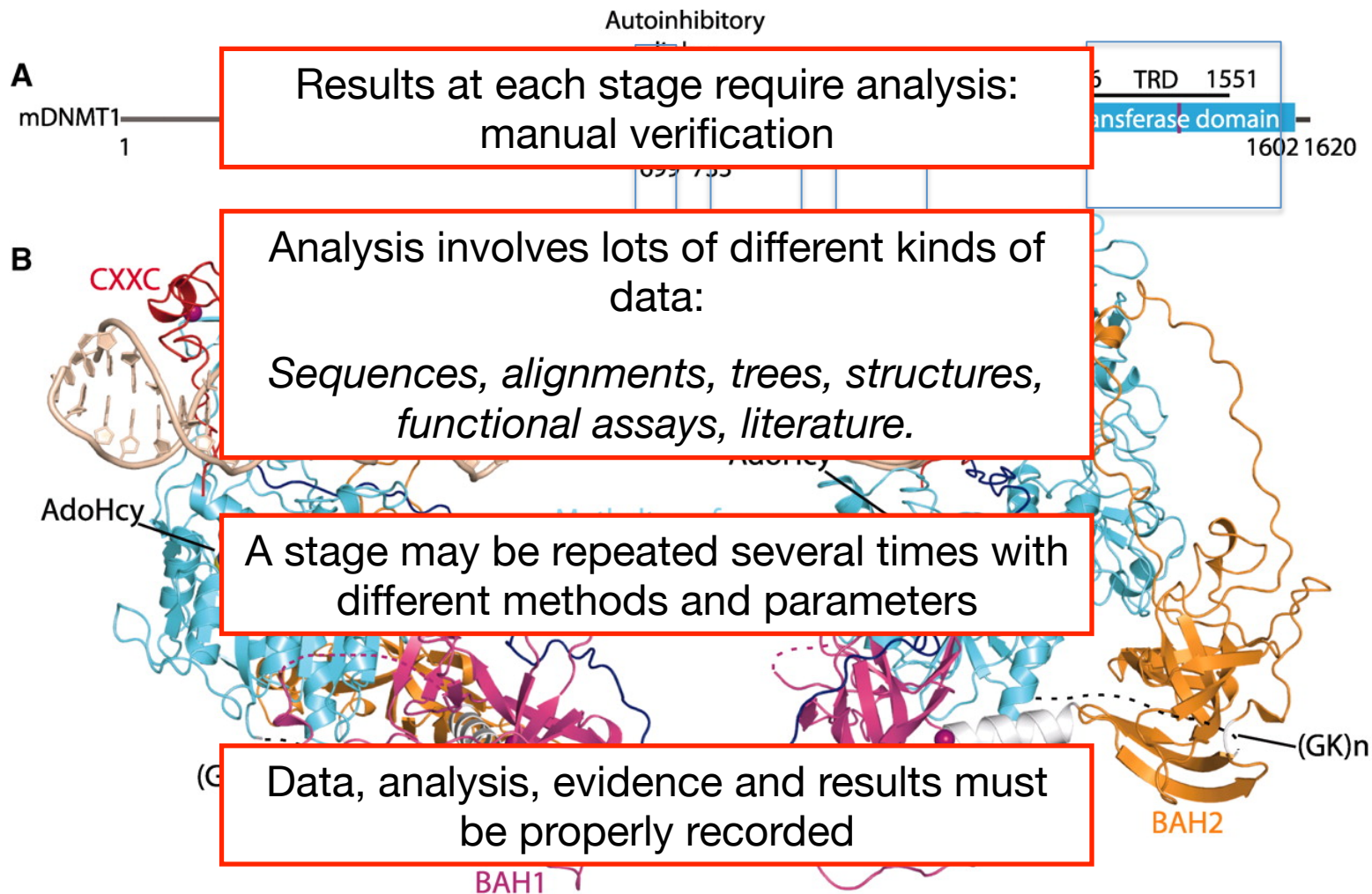


Fig. 1 Structural overview of mDNMT1(650–1602)–DNA 19-nucleotide oligomer complex with bound AdoHcy.

J Song et al. Science 2011;331:1036-1040

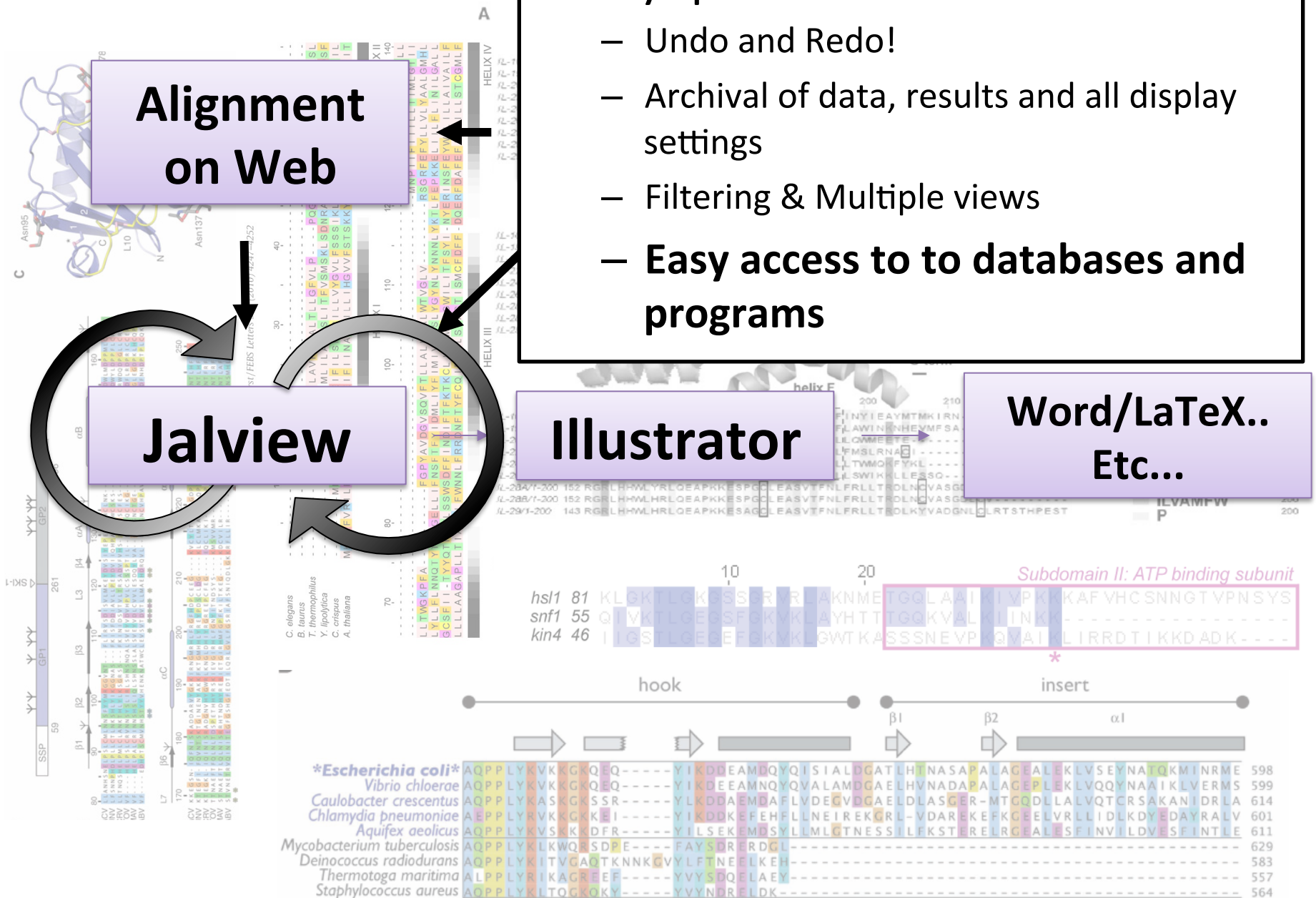
- Key qualities for a workbench
 - Undo and Redo!
 - Archival of data, results and all display settings
 - Filtering & Multiple views
 - Easy access to databases and programs

Alignment
on Web

Jalview

Illustrator

Word/LaTeX..
Etc...



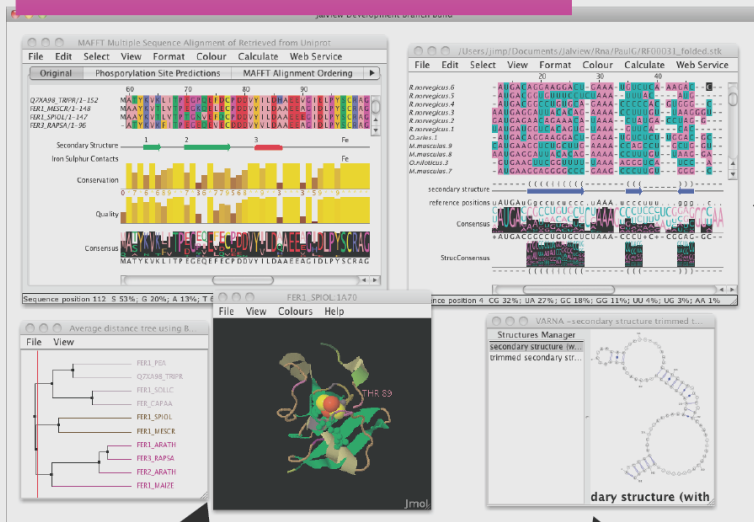
Jalview Flavours

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

Local
File
system

import
from web

Analysis Services

Protein 2ndary structure



Alignment Analysis

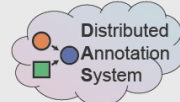
Protein Disorder

Multiple alignment



GLOBPLOT 2

Biological Data Services



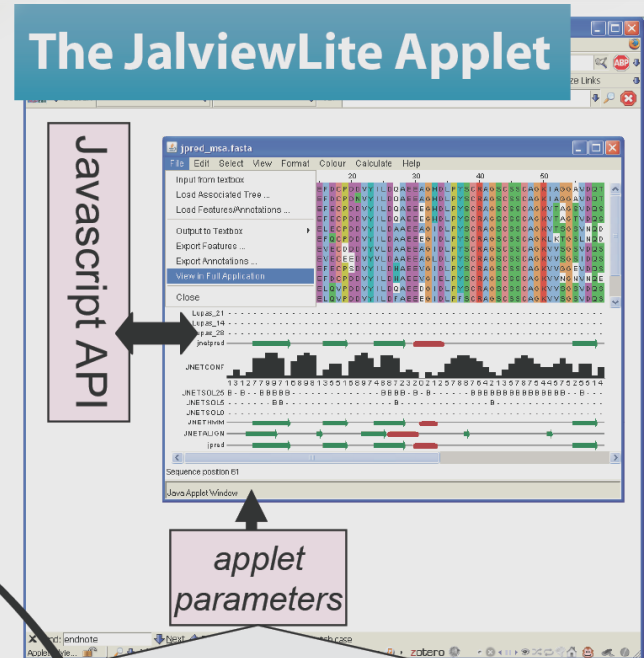
The JalviewLite Applet

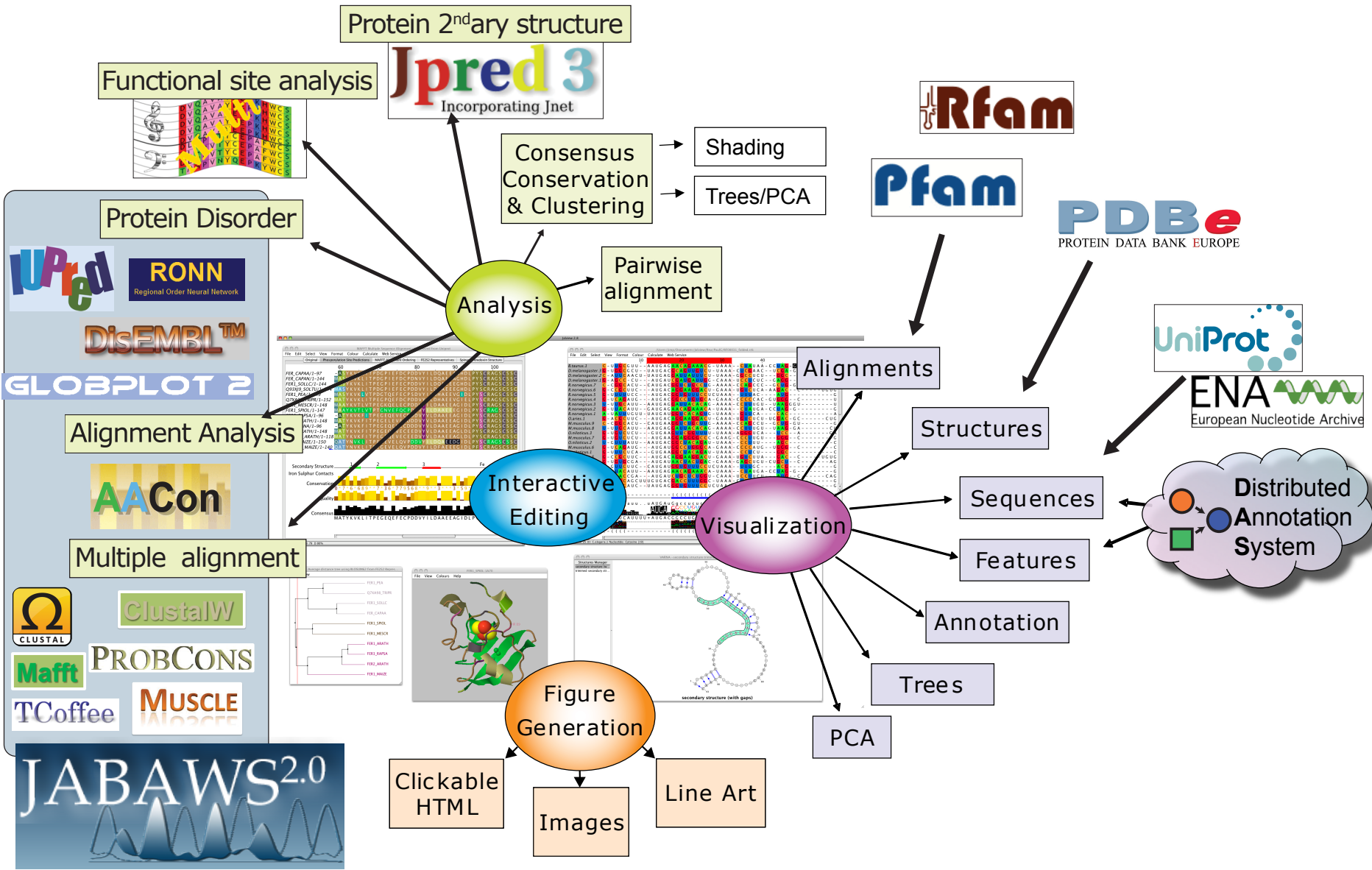
Javascript API

applet
parameters

Alignment
And
Annotation

Bioinformatics
Web Server







Jalview

Jalview
Launch
Buttons

Launch Jalview Applet

Launch Jalview Desktop

New logo

Home

About

Help

Community

Development

Training

Download

Latest News

Jalview in 2017 and 2013

Help and documentation

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

Installation packages and source

Jalview training news and course dates

Jalview Community

Jalview Development and release history

Registration now open for 3rd Jalview Residential Training Course and Hackathon
Posted On: 19-10-2012

TRAINING

Analysis Services



Biological Data Services



The Jalview Desktop

Javascript API

applet parameters

Alignment And Annotation

<http://www.jalview.org>

Launching the jalview desktop

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
FER1_MESCR/1-148
FER1_SPIOL/1-147
FER3_RAPSA/1-96
FER1_ARATH/1-14
FER_BRANA/1-96
FER2_ARATH/1-1
Q93Z60_ARATH/1
FER1_MAIZE/1-15

Secondar
Iron Sulphu
Co

Jalview

Version: 2.8

Last Updated: 06 February 2013
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

Sequence position

Average distance tree using B...

FER1_PEA
Q7XA98_TRIPR
FER1_SOLLIC
FER_CAPAA
PIOL
MESCR
ARATH
APSA
ARATH
MAIZE



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

Q7XA98_TRIPR/1-152
FER1_MESCR/1-148
FER1_SOLUC/1-148

60 70 80 90 100
M A T Y K V K L I T P E G Q E F E C P D D V Y I L D A A E E V G I E L P Y S C R A G S C S S
M A A Y K V T L V T P E G K Q E L E C P D D V Y I L D A A E E A G I D L P Y S C R A G S C S S
M A A Y K V T L V T P E G K Q E L E C P D D V Y I L D A A E E A G I D L P Y S C R A G S C S S

Average distance tree using B...

File View

FER1_PEA
Q7XA98_TRIPR
FER1_SOLUC

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

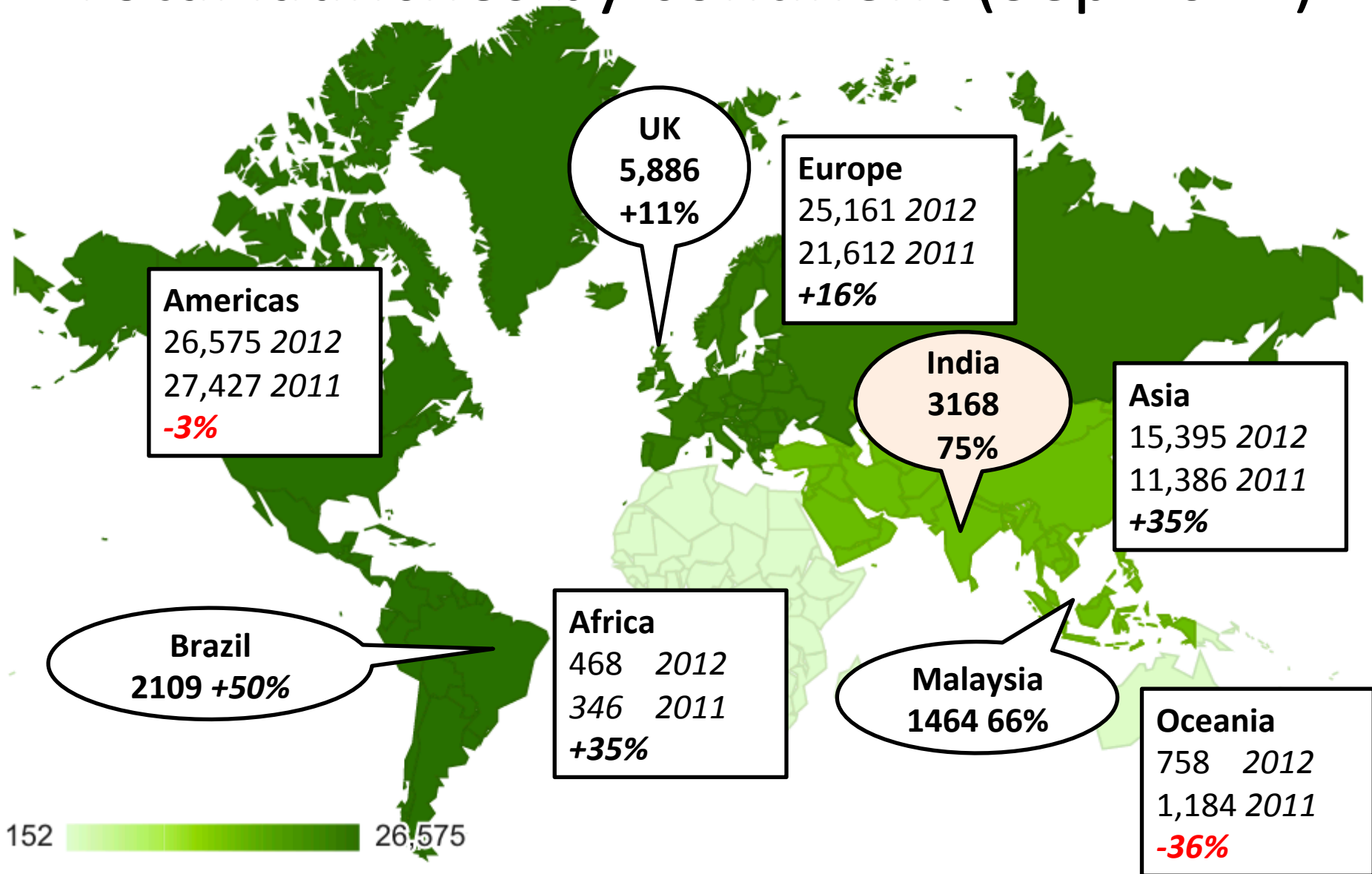
Quality
Consensus
M A Y K V K L I T P E G Q E F E C P D D V Y I L D A A E E V G I E L P Y S C R A G S C S S
M A T Y K V K L I T P E G Q E F E C P D D V Y I L D A A E E A G I D L P Y S C R A G S C S S

Sequence position 87 11.0



Jmol

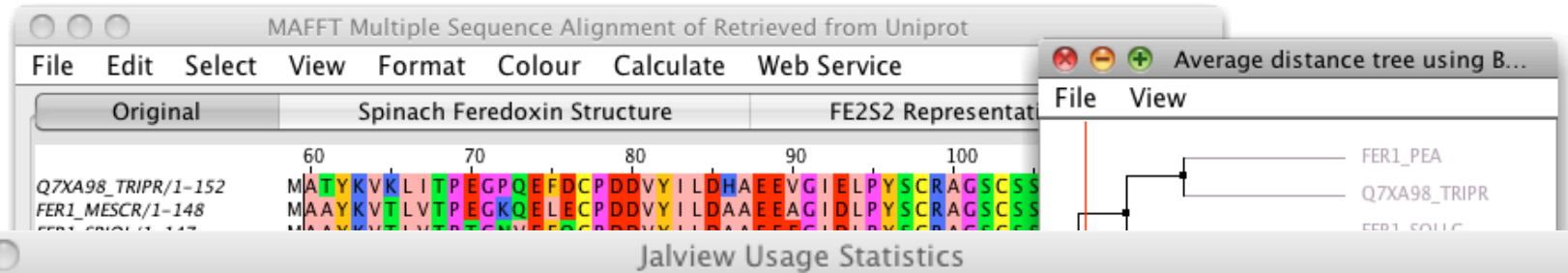
Total launches by continent (Sep 2012)



Jalview News



How accurate are the Google Analytics Launch Statistics ?



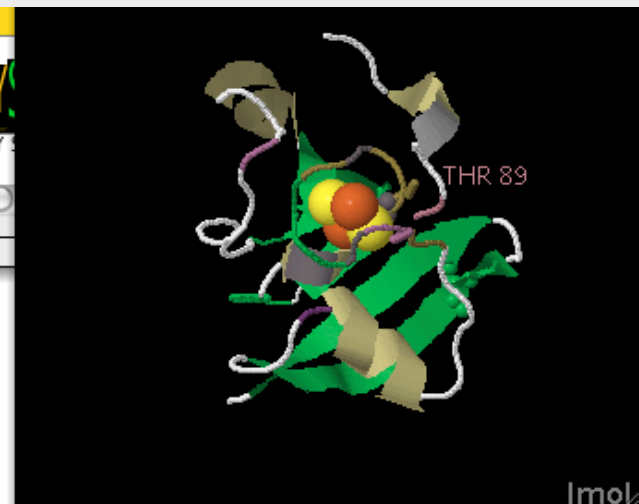
Do you want to help make Jalview better by enabling the collection of usage statistics with Google Analytics ?

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

Cancel

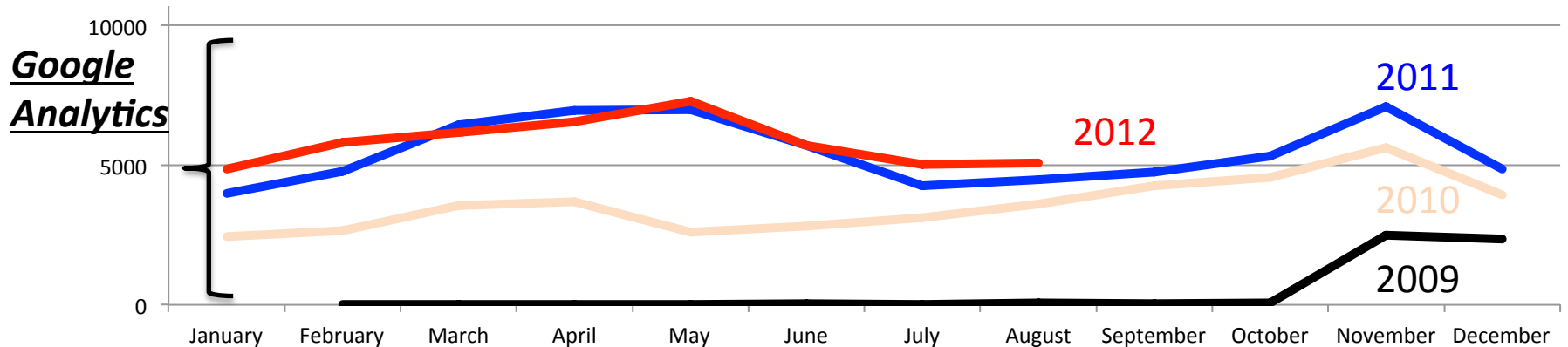
No

Yes

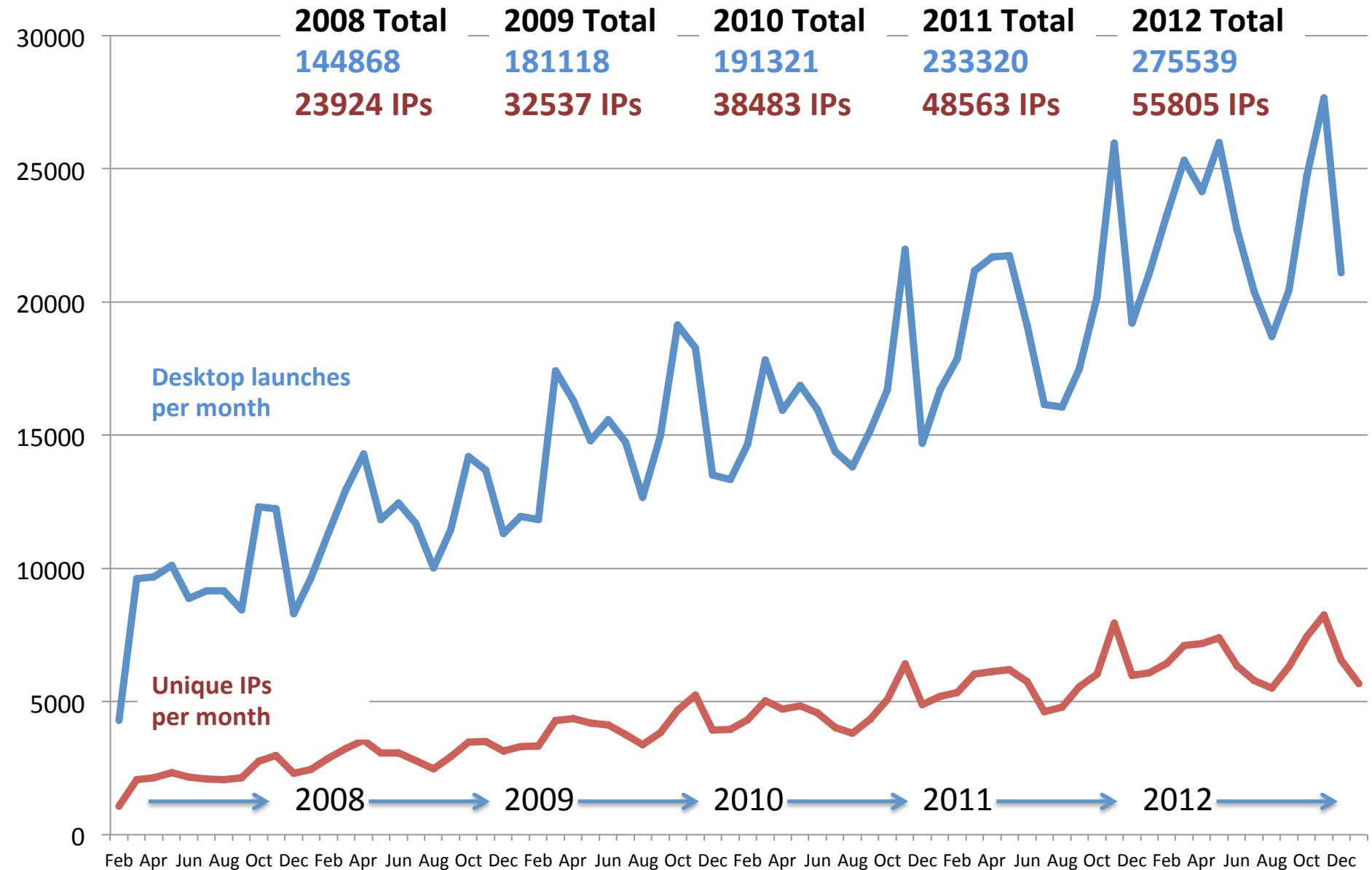


Year on Year increase in Desktop Launches as measured by Google Analytics vs our web server logs

1 in 4 users say 'no' to Google Analytics

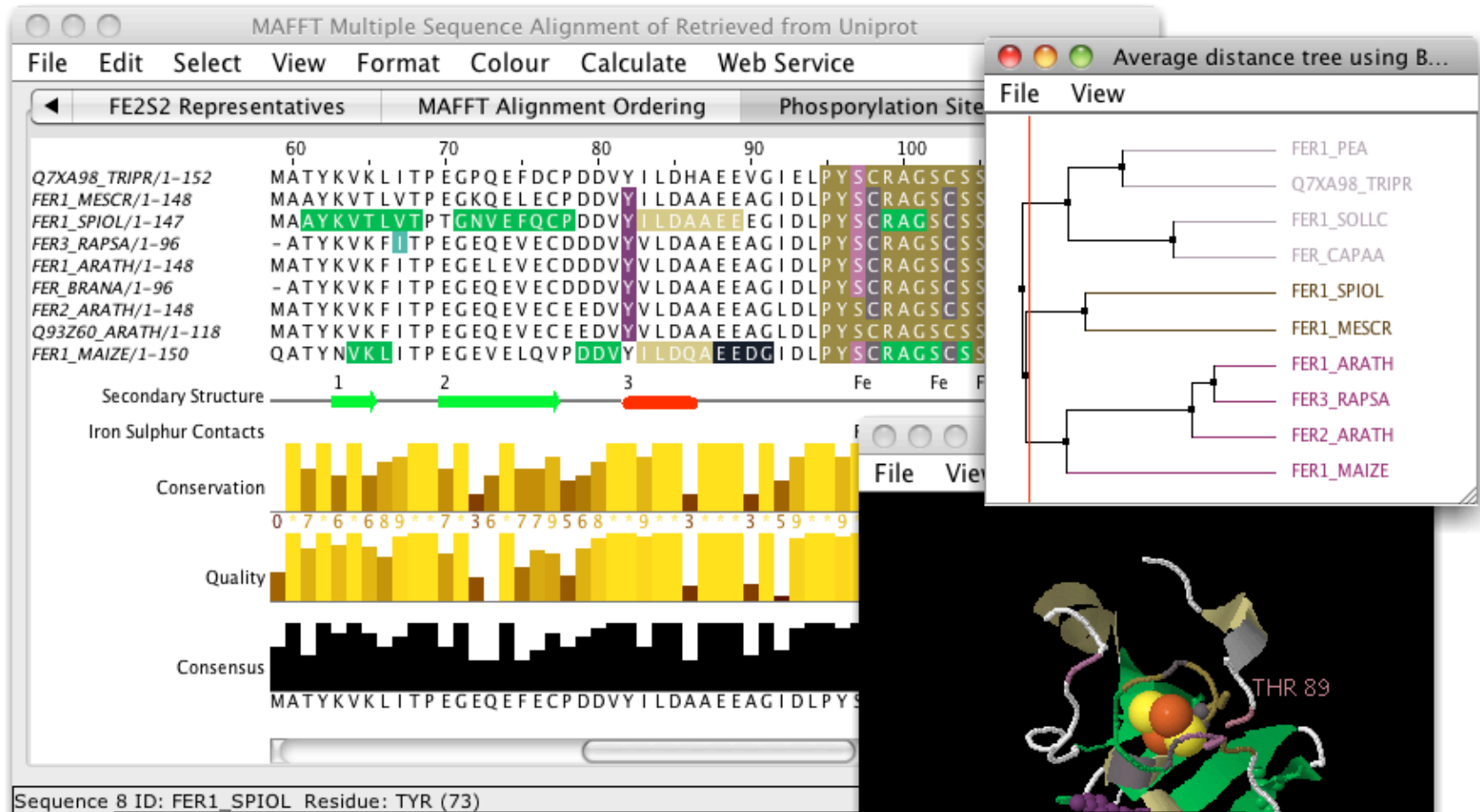


Jalview Desktop monthly usage from 2007-2012



The Jalview Example Project

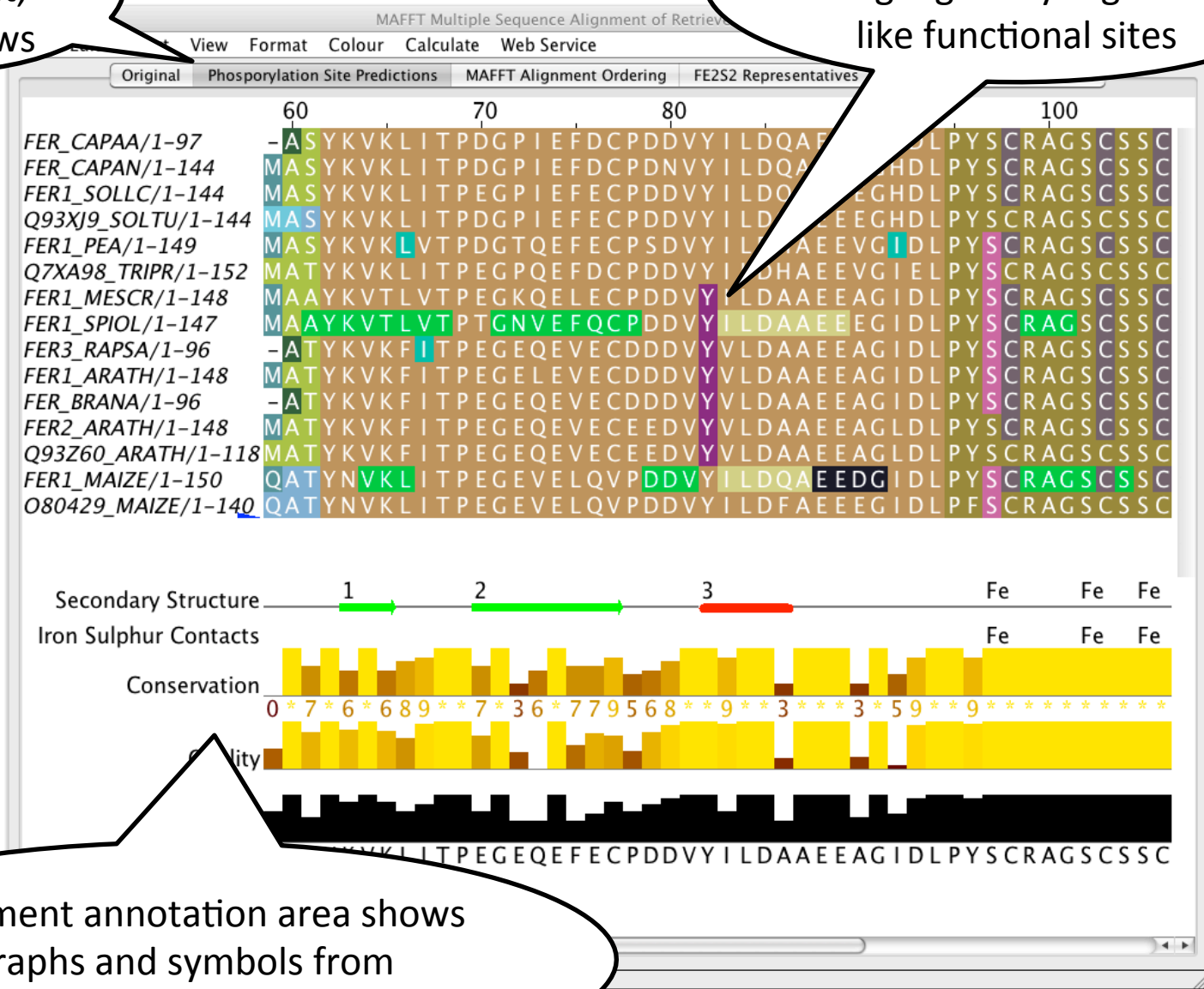
Jalview 2.8



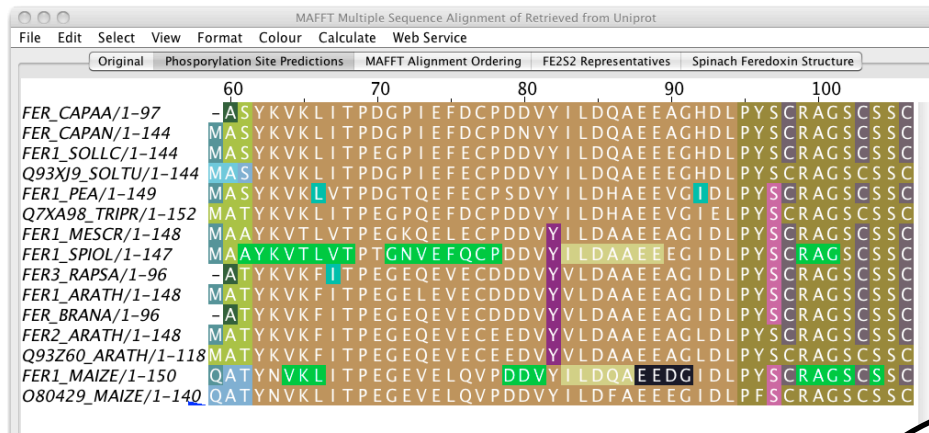
- Demonstrates most of Jalview's key features

One alignment, many views

Sequence features highlight key regions like functional sites

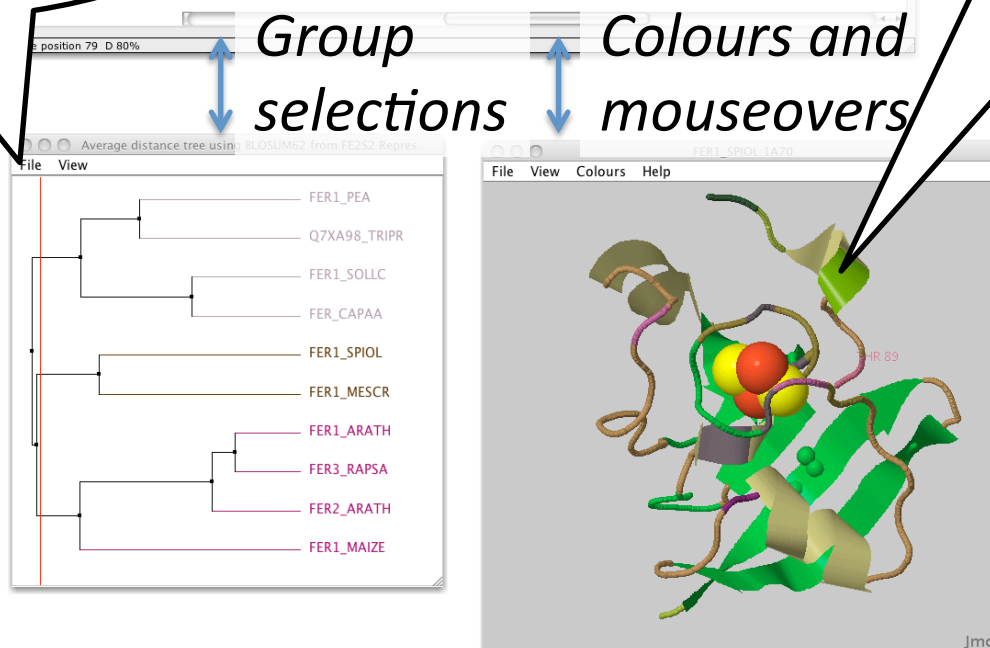


Alignment annotation area shows graphs and symbols from calculations and manual curation



Linked tree viewer
allows subgroups to
be identified in
alignment

Linked Jmol viewer
shows one or more
structures coloured by
alignment views



Typical jalview workflow

1. Import sequence or alignment
 - Drag/drop, Paste, or URL
2. Decorate sequences with references & annotation from external databases
3. Create alignment
4. Use built in shading, conservation analysis, tree and PCA capabilities to explore
 - Also use annotation and structure data if available
5. Select regions for refinement or further analysis
6. Import trees, annotation, etc. created with other programs to explore further
7. Prepare annotated views for publication

Phylogenetic analysis and Jalview

- **Built in tree methods**
 - UPGMA
 - Fast, simple, but not reliable for phylogenetic inference
 - Neighbour joining
 - Slower than UPGMA
 - Perhaps useful for a first approximation
 - Jalview's implementation is not the most efficient
- **Import trees for subgroup analysis**
 - Load any number of Newick/NH Extended files onto an alignment from another program
 - Bootstraps are displayed

Typical jalview workflow

1. Import sequence or alignment
 - Drag/drop, Paste, or URL
2. Decorate sequences with references & annotation from external databases
3. Create alignment
4. Use built in shading, conservation analysis, tree and PCA capabilities to explore
 - Also use annotation and structure data if available
5. Select regions for refinement or further analysis
6. Import trees, annotation, etc. created with other programs to explore further
7. Prepare annotated views for publication

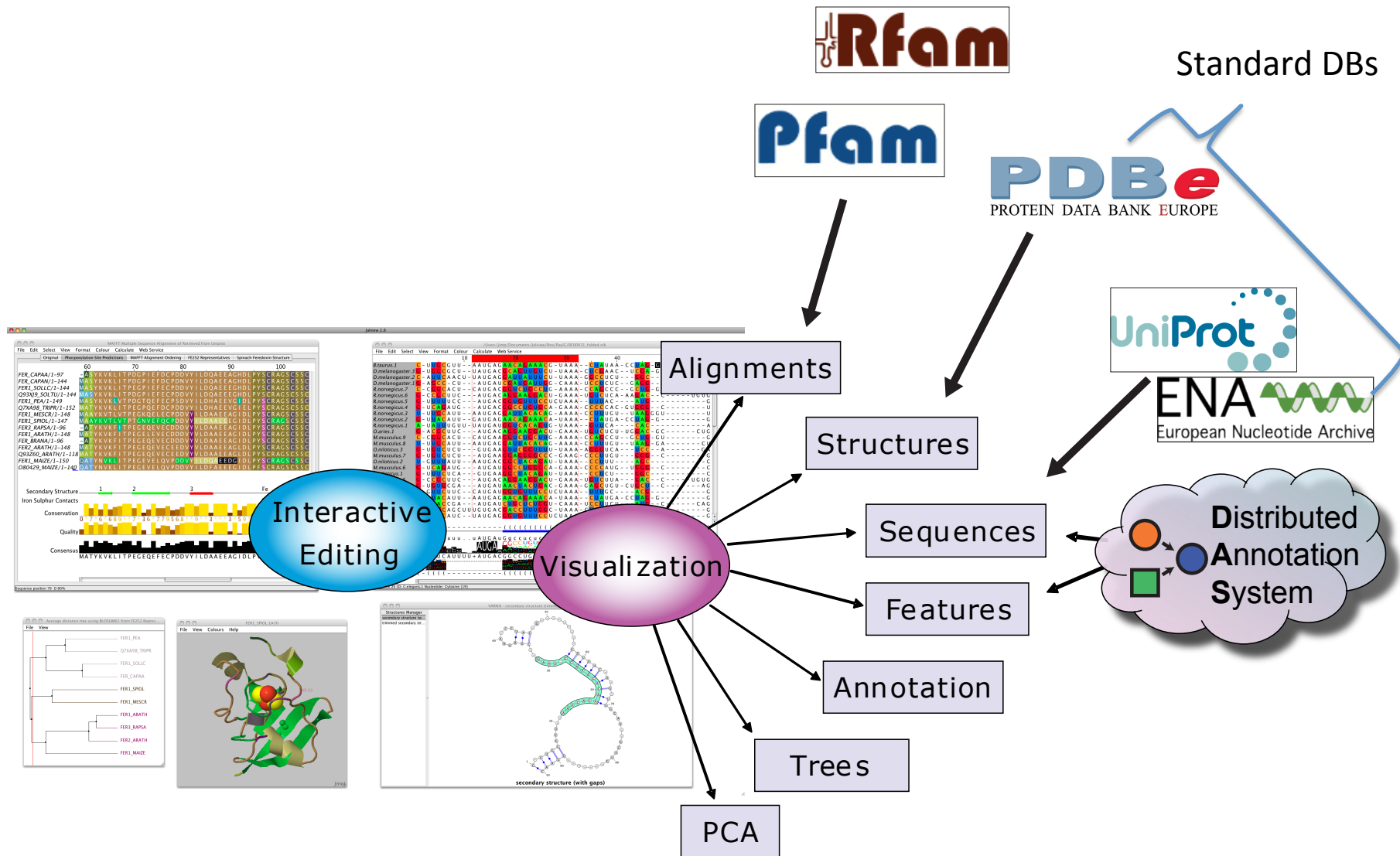
Save as
Jalview project
at strategic points



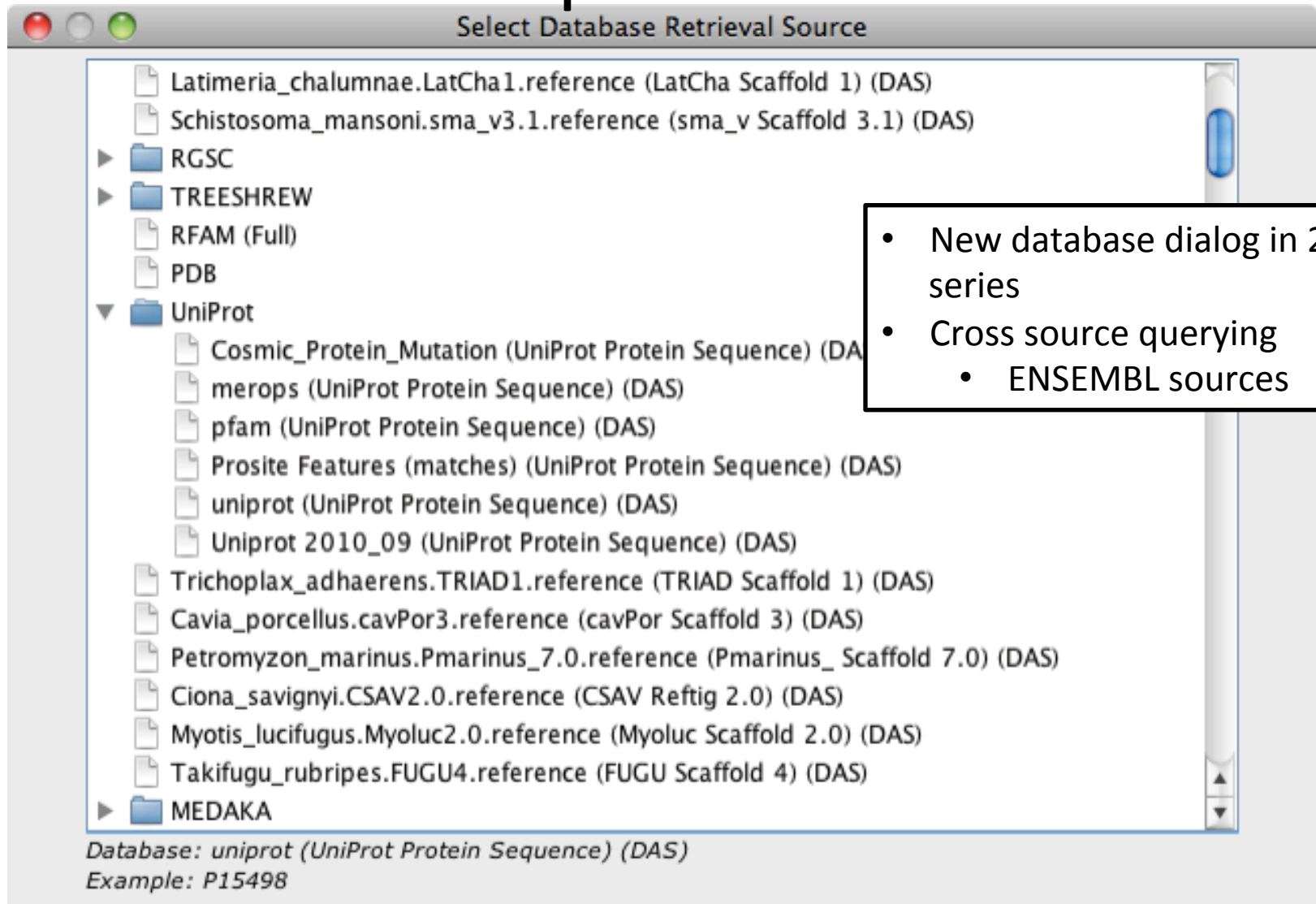
The screenshot displays the Jalview 2.8 software interface. The main window, titled 'MAFFT Multiple Sequence Alignment of Retrieved from Uniprot', shows a multiple sequence alignment of protein sequences. The sequences listed on the left include Q7XA98_TRIPR/1-150, FER1_MESCR/1-148, FER1_SPIOL/1-147, FER3_RAPSA/1-96, FER1_ARATH/1-148, FER2_ARATH/1-148, Q93Z60_ARATH/1-148, and FER1_MAIZE/1-150. The alignment is color-coded by amino acid type. Below the alignment, there are tracks for Secondary Structure (Iron Sulphur Contacts), Conservation (a bar chart), Quality (a bar chart), and Consensus. A smaller window titled 'Average distance tree using B...' shows a phylogenetic tree with the same sequences as labels. The bottom right corner of the image shows a 3D ribbon diagram of a protein structure with a label 'THR 89' and the Jmol logo.

- Jalview projects store key data for a session
 - Alignments
 - Annotation & Database IDs
 - Structures
 - Trees
 - Display settings
- New Jalview versions are tested for backwards compatibility
 - Archival record of your analysis

Retrieval from External Databases



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



Tip: Project owners, see our [Getting Started](#) guide for steps to configure your project. [X](#)

Project Information

 Recommend this on Google

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Code license

[Apache License 2.0](#)

Labels

[DAS](#), [JDAS](#)

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[jdass-1.0.1.jar](#)
[jdass-1.0.2.jar](#)
[Show all »](#)

JDAS is a Java DAS client library which simplifies DAS queries and maps Java classes to DAS XML representations. JDAS includes JAVA classes generated from DAS RNG schemas. These Java classes are used through the JAXB API to store and retrieve data in memory without the need to implement a specific set of XML loading and saving routines. JAXB provides two main features: the ability to marshal Java objects into XML and the inverse, to unmarshal XML into Java objects. JDAS additionally implements adaptor classes which are used to refactor generated classes with a complex structure. Finally JDAS implements client classes to facilitate querying DAS information.

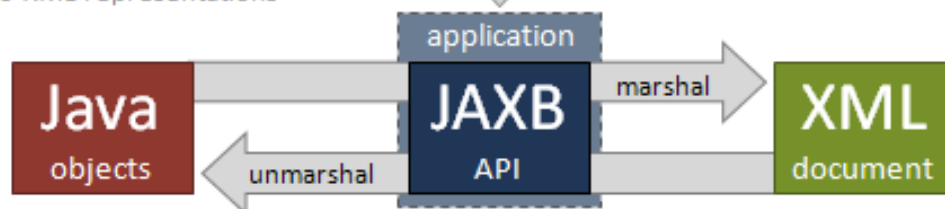
Developed by Rafael Jiminez,
Jonathan Warren and other Java
developers in DAS Community

[Table Of Contents](#)

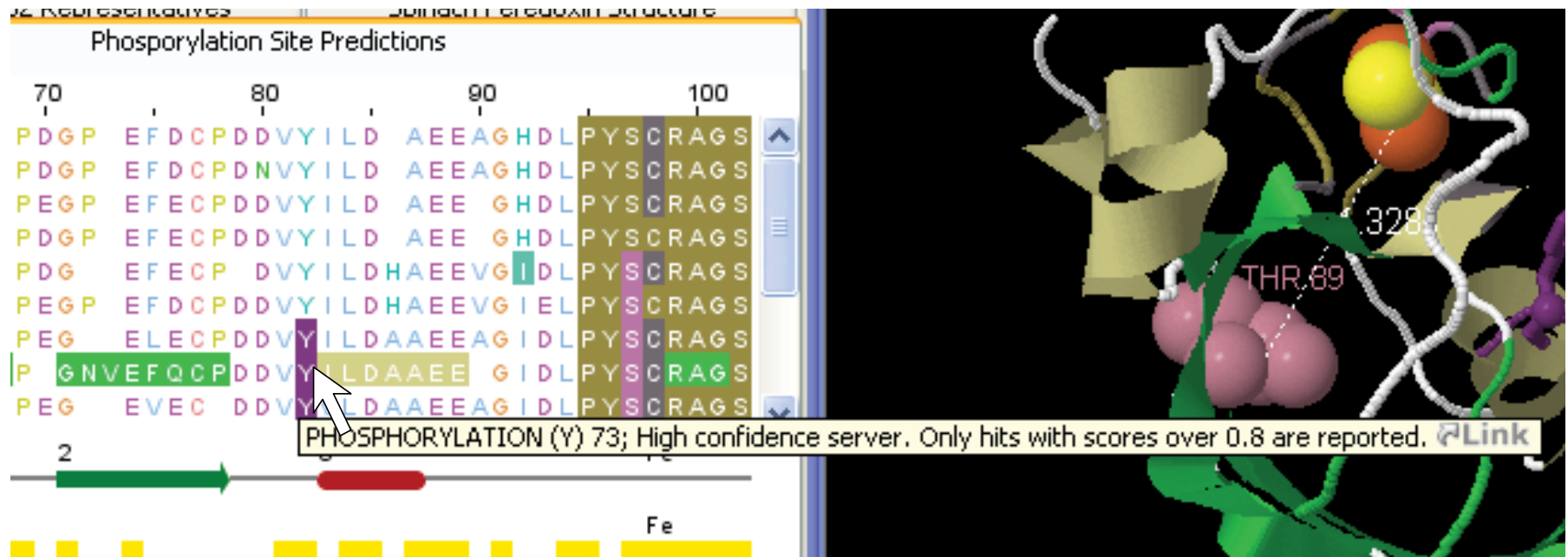
Java classes representing the DAS schema



Mapping Java classes to XML representations



Sequence Features



Sources of sequence feature data

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

Sequence Features Dialog box

The diagram illustrates the 'Sequence Feature Settings' dialog box, which is used to configure sequence features. A central cloud labeled 'DAS ANNOTATION SERVERS' is connected to various parts of the dialog by arrows, indicating its role in providing data and annotations.

Sequence Feature Settings Dialog Box Components:

- Feature Settings Tab:**
 - 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:** (http://www.dasregistry.org/dasregistry/coordsys/CS_D56) Protein Sequence, UniProt
- Feature List:**
 - uniprot:** ☒ (Selected)
 - PDBsum_protprot:** ☒ (Selected)
 - Pfam Other Features:** ☐ (Not selected)
 - chs_total:** ☒ (Selected)
- Feature Type Table:**

Feature Type	Colour	Display
DISULFID		☒
Protein-protein contact		☒
MOD_RES		☒
ISOFORM		☒
PHOSPHORYLATION (S)		☒
PHOSPHORYLATION (Y)		☒
INIT_MET		☒
PHOSPHORYLATION (T)		☒
ES-SIGNAL		☒
CONFLICT		☒
ACETYLATION		☒
TURN		☒
HELIX		☒
STRAND		☒
SIGNAL		☒
COMPLEX		☒
PROSITE		☒
PRINTS		☒
PROPEL		☒
OUTSIDE		☒
CHAIN		☒
Pfam		☒
ProDom		☒
- Buttons:**
 - Fetch DAS Features:** (Bottom left)
 - Refresh Available Sources:** (Bottom left)
 - Add Local Source:** (Bottom left)
 - Invert Selection:** (Bottom right)
 - Load Colours:** (Bottom right)
 - Save Colours:** (Bottom right)

Annotations and Interactions:

- Cloud:** DAS ANNOTATION SERVERS
- Arrows:**
 - From cloud to 'Filtered list' and 'Add user defined sources'.
 - From cloud to 'Group features by source' and 'Type==colour'.
 - From cloud to 'Highlight start-end' and 'Order for optimal display'.
 - From cloud to 'Query matches ID to Authority' and 'Map to local reference frame'.
 - From cloud to 'Mouse over for feature name, links and scores'.

Sequence Data (Bottom):

```

UniProt/Swiss-Prot|P17870P - - PNL - PCSV - - DTGK - - GVD - EVKAPCAENL - -
UniProt/Swiss-Prot|P51485A - - PKS - ASSV - - DTGK - - GVD - EVKAPCAENL - -
UniProt/Swiss-Prot|P51487P - - PNS - PPSV - - DD LGK - - GVEYTIRAYVADSE - -
UniProt/Swiss-Prot|P51484P - - ENA - PPSV - - DD LGK - - GVEYTIRAYVADSE - -
UniProt/Swiss-Prot|P32122P - - ASS - PPSV - - DD LGK - - GVEYTIRAYVADSE - -
UniProt/Swiss-Prot|P08168P - - DYL - PCSV - - DD LGK - - GVEYTIRAYVADSE - -
UniProt/Swiss-Prot|P53179P - - PRGR - LSI - - - - - - KFERG - - SITYFLSCTLESNNI - -
UniProt/Swiss-Prot|Q09889P - - PDI - PDSI - - - - - - EGIPGCHI IYTLTASLERATQ - -
UniProt/Swiss-Prot|P30647P - - LNC - PPSY - - - - - - ESQFG - - SIRYQMKVELRASTD - -
UniProt/Swiss-Prot|O45782P - - KSL - PPSF - - - - - - EGEFG - - HIRYTKAICERPWD - -
UniProt/Swiss-Prot|O76685P - - INV - PPSF - - - - - - EGKYG - - YLRY - - SVTA EVD RPWR - -
UniProt/Swiss-Prot|O17812P - - ENI - PQSF - - - - - - EGPGF - - FIRFYIKVHMDRPHA - -
  
```

Shading, thresholding, colour by label.

... MASTALSSAIVSTSFLLRRQQTPISLRSLPFANT... QSLFGLKS... STARGGRVTAMATYKVKELTPDG...
... MAATTTTMMGMATTFVPKPQAPPMMAALPSNTG... RSLFGLKT...
... MASISGTMISTSFLLPRKPAVTSLKAI... NVG... EALFGLKS...
... MASTALSSAIVSTSFLLRRQQTPISLRSLPFANT... QSLFGLKS...
... MASISGTMISTSFLLPRKPVVTSLKAI... NVG... EALFGLKS...
ATVLGSPRAPAFFSSSLRAAPATAVALPAAKVG... IMGRSA...
... MASVSATMISTSFMPRKPAVTSLKPI... NVG... EALFGLKS...
... MATTPALYGTAVSTSFMRQPVPMVSVATT... TTKAFPSGFGGLKSV...
... MAATTAALSGATMSTAFAPKT... PPMTAALPTNVG... RALFGLKS...
... MASTALSSAIVGTSFIRRSAPISLRSLPSANT... QSLFGLKS...
... MAATALSMSILRAP... PCFSSPLRLRVAVAKPLAAPM...
... MATTPALYGTAVSTSFLLRTQPMPSVTTTKAF... SN... GFLGLKT... SLK...

Graduated Feature Colour for hydrophobic_region

☐ Colour by Label Min: Max:

No Threshold ☐ Threshold is Min/Max

Feature Type	Colour	Display
metal ion-binding site		☒
O-phosphorylated L-serine		☒
O-phosphorylated L-threonine		☒
O4'-phosphorylated L-tyrosine		☒
hydrophobic_region		☒

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

... MMAS+ALSGT+VSTSFLLRRQPAPTSLAALP+NVG... +SLFGLKS... STA...
VYILDQAEAEAGHDLPPYSCRAGSCSSCAGKIAGGAVDQTDGNFLDDQLE...
VYVLDAAEEAGLDLPYSCRAGSCSSCAGKVVSGSIDQSDQS... LDD...
VYILDQAEAEAGHDLPPYSCRAGSCSSCAGKLTSLND... S... DDID...
VYILDQAEAEAGHDLPPYSCRAGSCSSCAGKVTAGVDDQSDGNFLDDQEA...
VYVLDAAEEAGIDLPYSCRAGSCSSCAGKVVSGSVDQSDQSFLLDDQIA...
VYVLDAAEEAGLDLPYSCRAGSCSSCAGKVVSGSIDQSDQS... LDD...EQME...
VYILDQAEAEAGHDLPPYSCRAGSCSSCAGKVTAGTVDDQSD... FLDDQEA...
VYILDQAEEDGIDLPYSCRAGSCSSCAGKVVSGSVDQSDQSYLDDGQIA...
VYILDQAEAEAGHDLPPYSCRAGSCSSCAGKIAGGAVDQTDGNFLDDQLE...
VYILDHAEVEGIDLPYSCRAGSCSSCAGKVVNGNVNDEDS... LDD...EQIE...
VYVLDAAEEAGIDLPYSCRAGSCSSCAGKVVSGFVDDQSDSFLDDQIA...
VYILDQAEAEAGIDLPYSCRAGSCSSCAGKVTSGSVNDDQDS... LDD...QDI...
VYVLDAAEEAGIDLPYSCRAGSCSSCAGKVVSGSVDQSDQSFLLDDQIE...
VYILDFAEEEGIDLPYSCRAGSCSSCAGKVVSGSVDQSDQSFLLNDQVA...
VYILDHAEVEGIDLPYSCRAGSCSSCAGKVVGGVDDQSDGSFLDDQIEAGFVLT... CVAYPTSDVVIETH

Clustal Omega quick alignment of millions of sequences



ClustalW

Mafft

PROBCONS

TCoffee

MUSCLE

Jpred 3
Incorporating Jnet

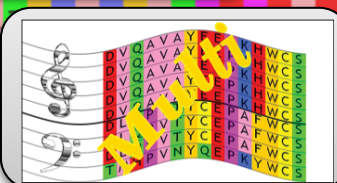
RONN
Regional Order Neural Network

DisEMBL™

UPred

GLOBPLOT 2

Assorted protein disorder predictors



Protein conservation calculations

AACon

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

JABAWS 2 services
in Jalview 2.8

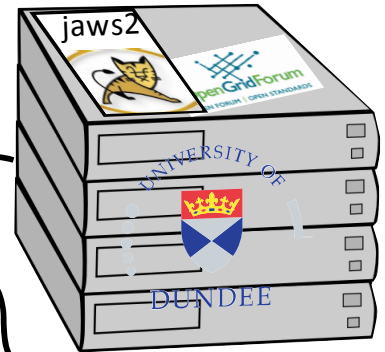
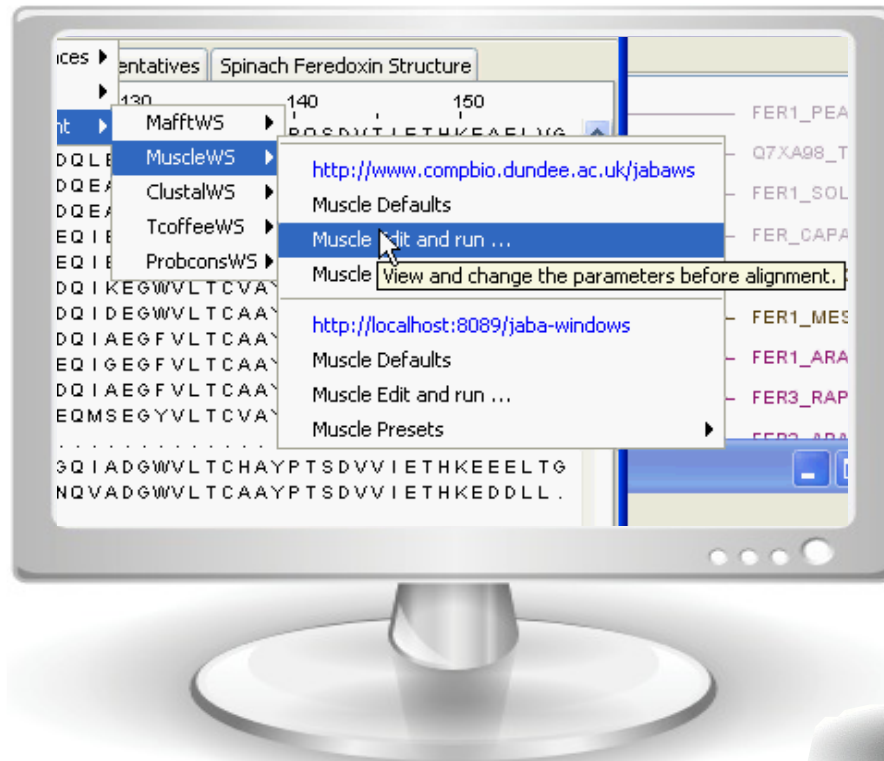
Alignment Web Services: JABAWS:MSA

Replaces original Jalview 2 services:

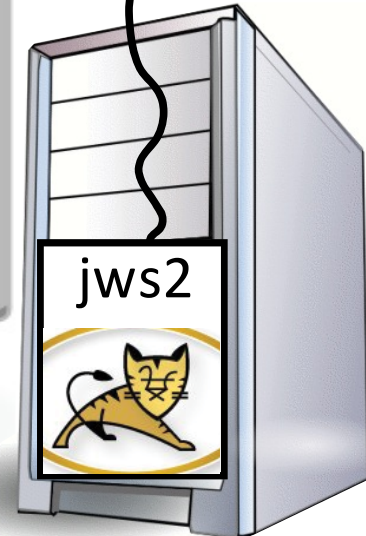
- Extensible framework for wrapping command line programs
- Can be installed on user's own machine/cluster

See Troshin et al. application note in *Bioinformatics* for more details.

Peter Troshin



HTTP



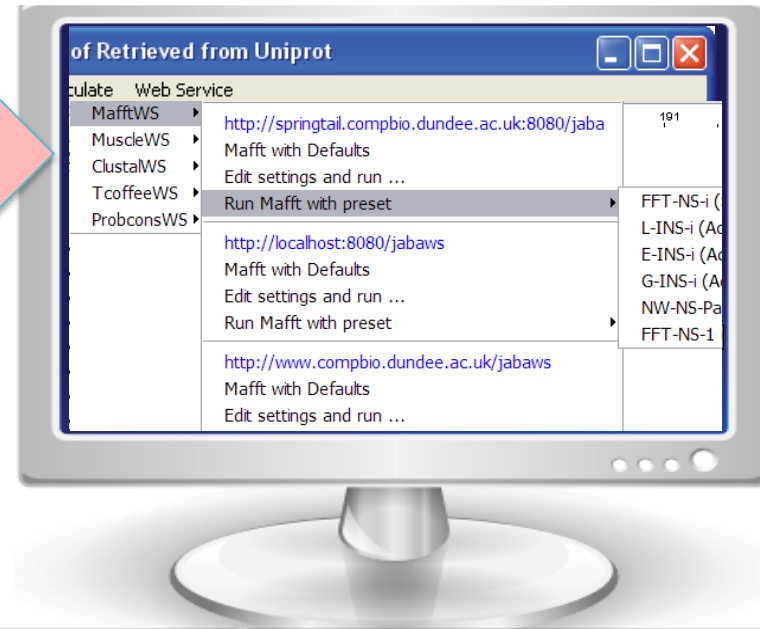
www.compbio.dundee.ac.uk/jabaws

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

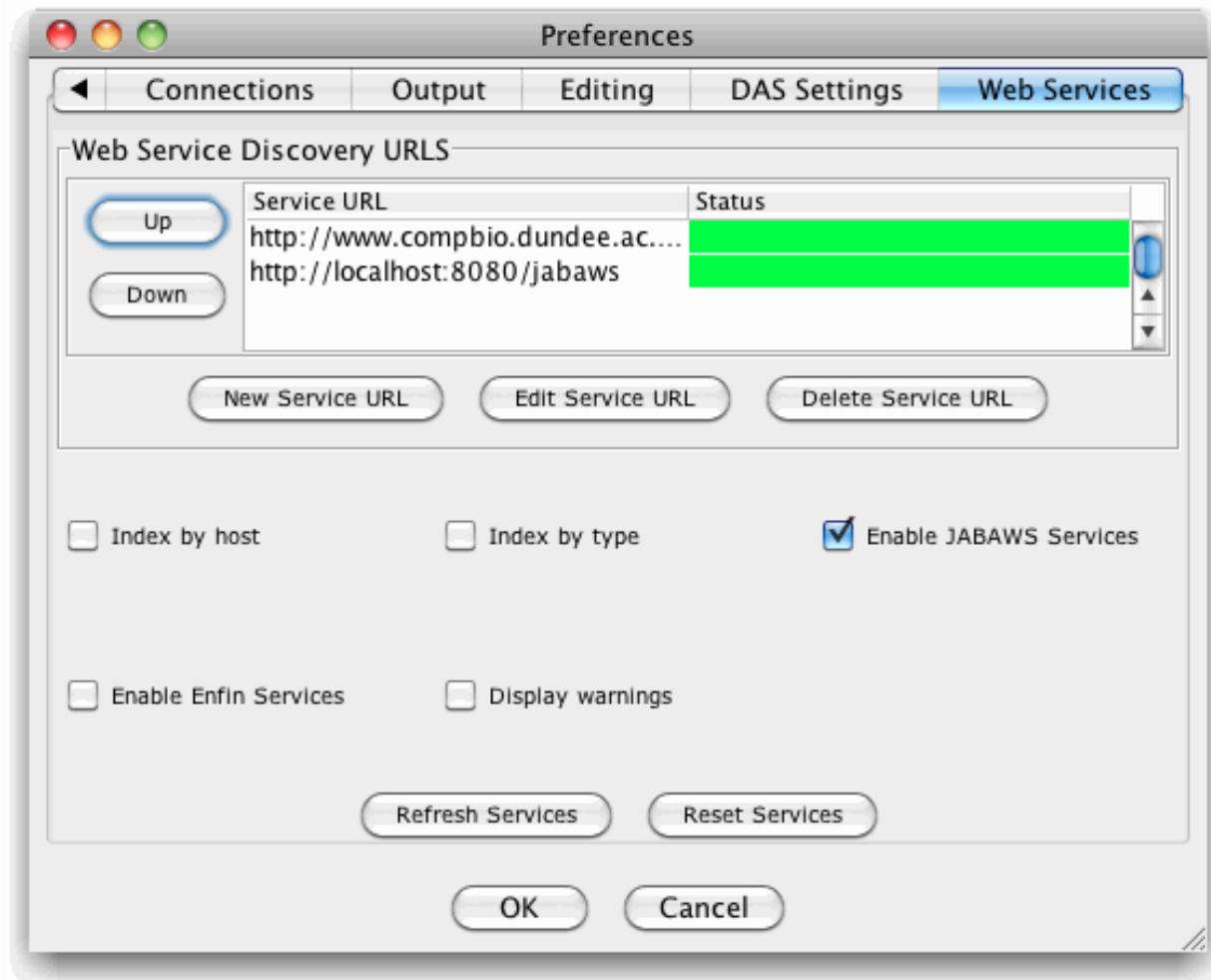


JABAWS Amazon
Machine Image
on EC2

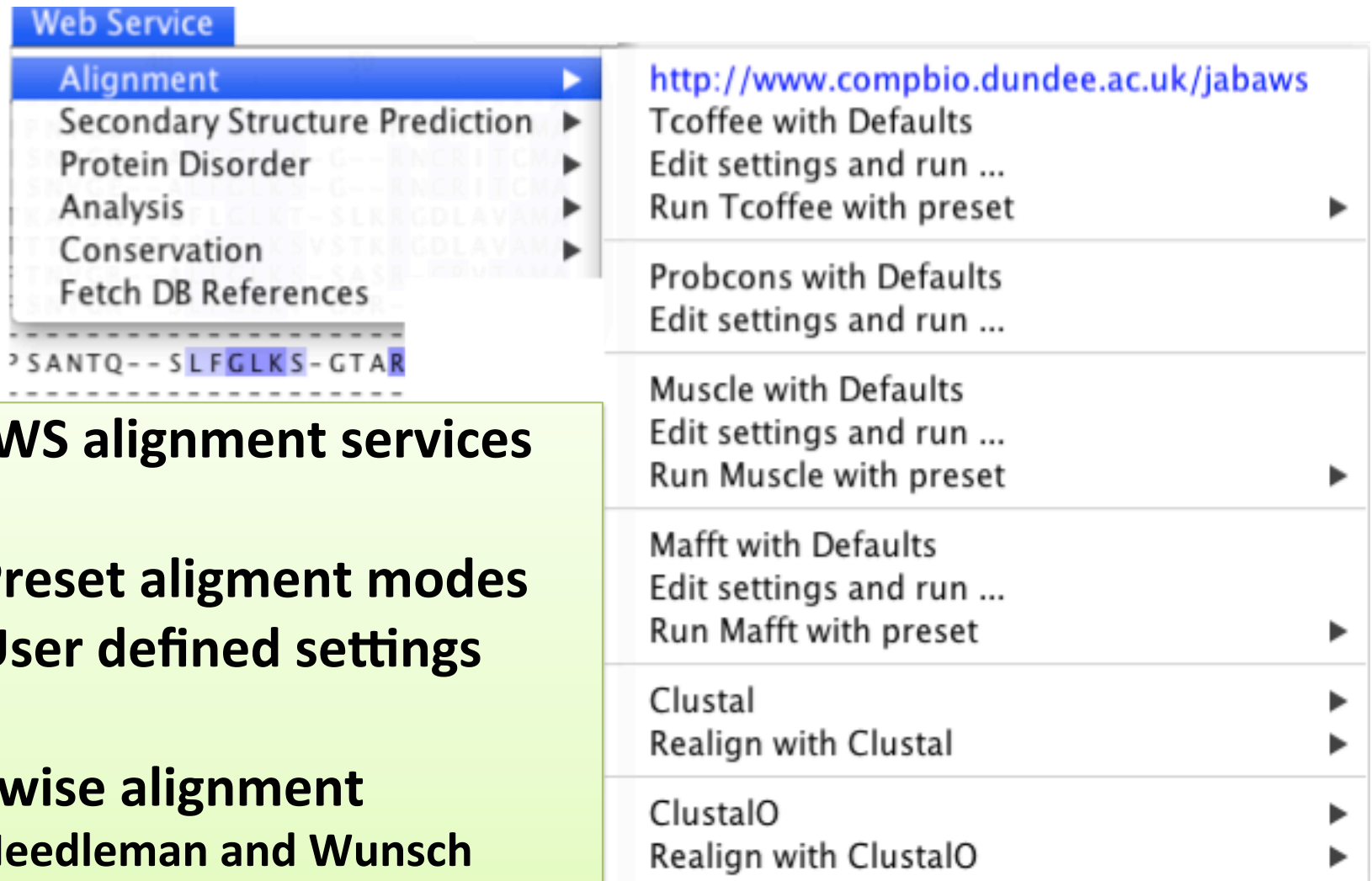


the
cloud
market

Jalview's JABAWS Configuration Panel



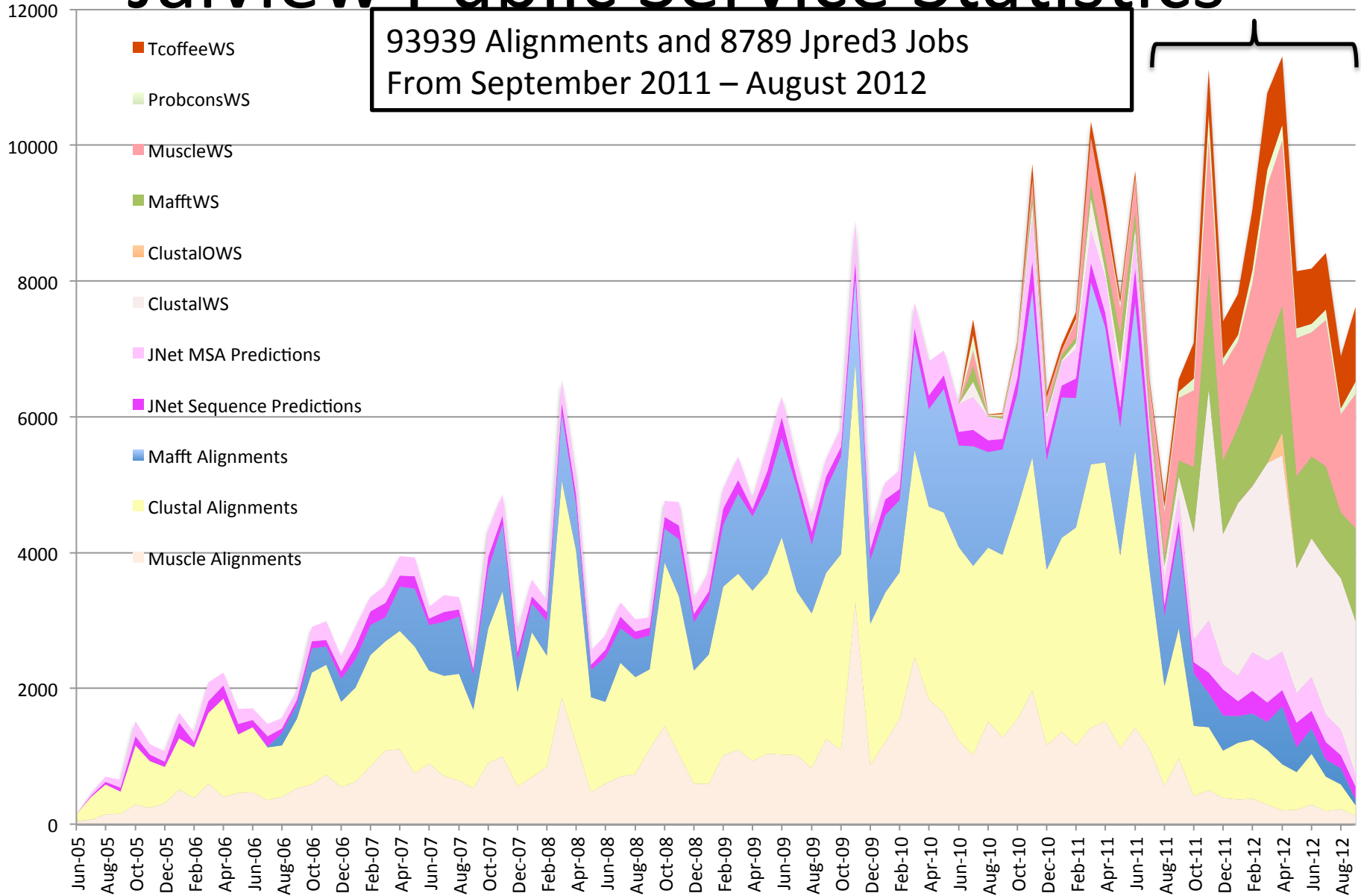
Jalview's Alignment Methods



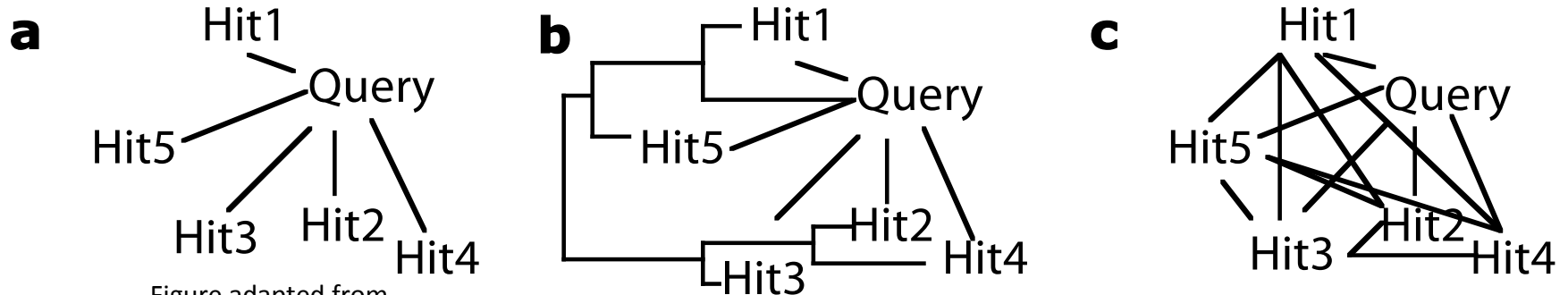
- **JABWS alignment services**
 - Preset alignment modes
 - User defined settings
- **Pairwise alignment**
 - Needleman and Wunsch
 - Mostly used internally

Jalview Public Service Statistics

93939 Alignments and 8789 Jpred3 Jobs
From September 2011 – August 2012



Common types of alignment algorithm



- a. Sequence database searches – optimal alignment between query and hit
e.g. **Blast** (single sequence), **PSI-Blast** and **HMMER**
- b. Progressive – optimise alignment between branches on guide tree
e.g. **ClustalW**
- c. 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**, are hybrids – employ sampling strategies to speed up tree building & refinement.

Alignment Job Parameter Settings

The screenshot shows a dialog box titled "Edit parameters for Align with MuscleWS". It contains several sections: "Details", "Options", "Parameters", and "Maxiters".

- Details:** A text box for adding notes for the parameter set.
- Options:** A list of checkboxes for "dimer", "Diagonal", "Diagonal 1", and "Profile scoring method". The "Profile scoring method" is checked.
- Parameters:** A section containing a "Sequence type" dropdown menu set to "auto".
- Maxiters:** A dropdown menu at the bottom right.
- Buttons:** "Revert", "Create", "Start Job", and "Cancel Job".

Callouts provide additional information:

- "Browse or edit to change name of set" points to the "Current parameter set name" dropdown, which is set to "User Defaults".
- "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.
- "Tooltips give brief description and link (right click) to further info" points to a tooltip for the "Profile scoring method" checkbox, which describes the "le" (log-expectation profile score VTM240) and "sp" (sum-of-pairs protein profile score) options and includes a "Link" button.

‘Realignment’ – adding sequences to an existing alignment



Clustal Realign options:

- Jalview leaves gaps in when sending sequences to JABAWS
- ClustalW
 - Fixes sequences with gaps, aligns other sequences to profile
- ClustalO
 - Creates an HMM from sequences with gaps
 - Aligns all sequences to HMM

Clustal Omega quick alignment of millions of sequences



ClustalW

Mafft

PROBCONS

TCoffee

MUSCLE

File Edit Select View Format Colour Calculate Web Service

MAFFT Alignment Ordering

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
Q7XA98_TRIPR/1-152	MATYKVKL	ITPEGPQEF	DCPDDVY		
FER1_MESCR/1-148	MAAYKVT	LVTPGKQEL	ECPPDDVY		
FER1_SPIOL/1-147	MAAYKVT	LVTPGNVEF	QCPDDVY		
FER3_RAPSA/1-96	-ATYKVKF	ITPEGEQEVE	CDDDVY		
FER1_ARATH/1-148	MATYKVKF	ITPEGELEVE	CDDDVY		
FER_BRANA/1-96	-ATYKVKF	ITPEGEQEVE	CDDDVY		
FER2_ARATH/1-148	MATYKVKF	ITPEGEQEVE	CEEDVY		

Secondary Structure

Iron Sulphur Contacts

AACon

Alignment

Secondary Structure Prediction

Protein Disorder

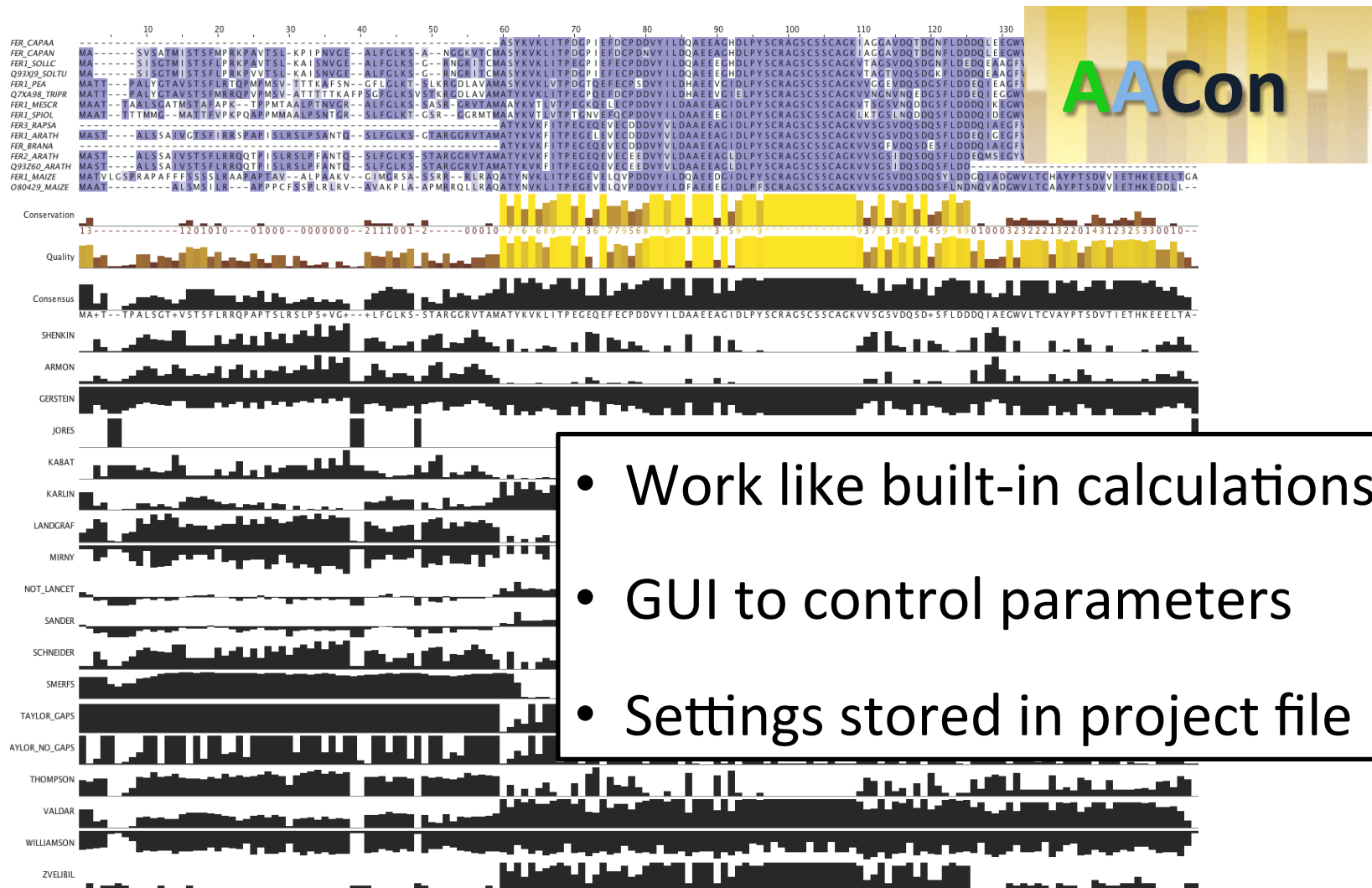
Analysis

Conservation

Envision 2

Fetch DB References

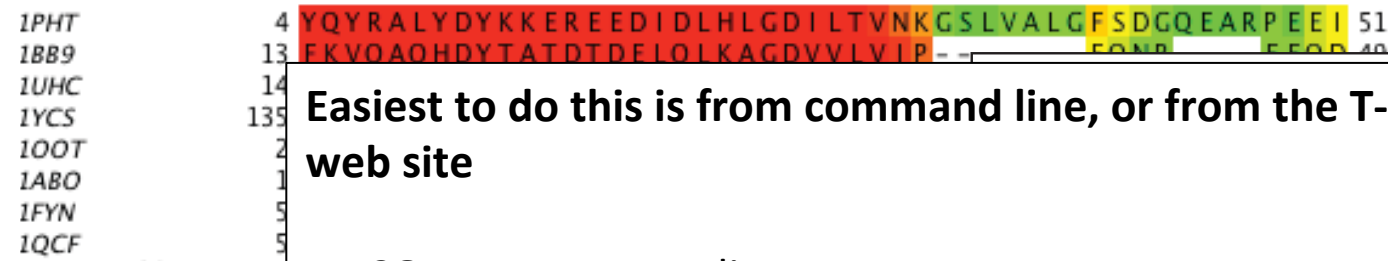
18 new alignment conservation calculations provided as web services



Are conservation scores trustworthy ?

- Good quality alignments
 - Conservation == probable molecular similarity
- Poor alignments
 - Conservation == random noise
- How do you measure MSA reliability ?
 - Try different methods. Vary parameters
 - Compare the results.

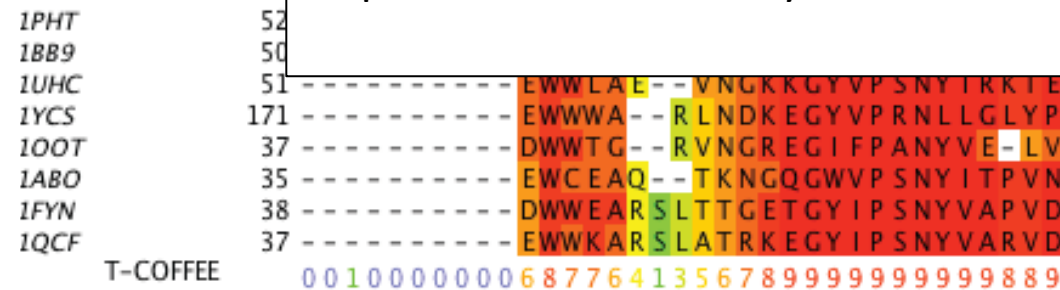
T-COFFEE alignment reliability scores



Easiest to do this is from command line, or from the T-COFFEE web site

- **CORE** – score an alignment
 - <http://tcoffee.crg.cat/apps/tcoffee/do:core>
- **M-COFFEE** – combine results from many ‘popular aligners’
 - <http://tcoffee.crg.cat/apps/tcoffee/do:mcoffee>
- Jalview can read the ‘score_ascii’ file for an alignment

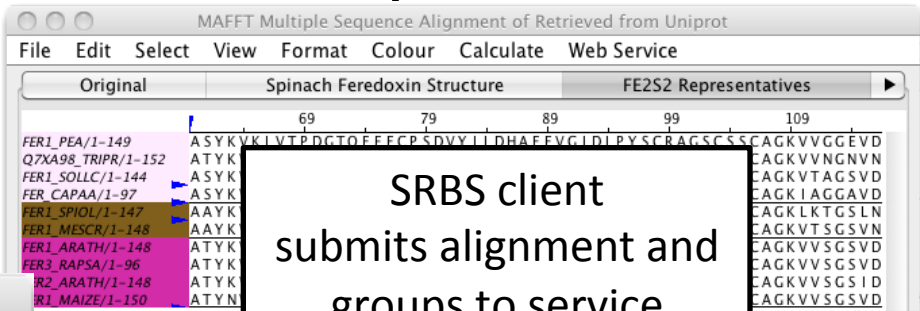
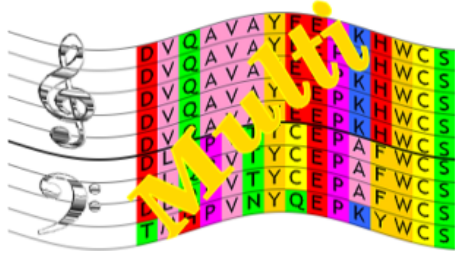
Hope to add functionality to JABAWS in future



es
nment
OFFEE
reliable
blue.

Help





SRBS client
submits alignment and
groups to service

i Paste in your alignmer

exampl

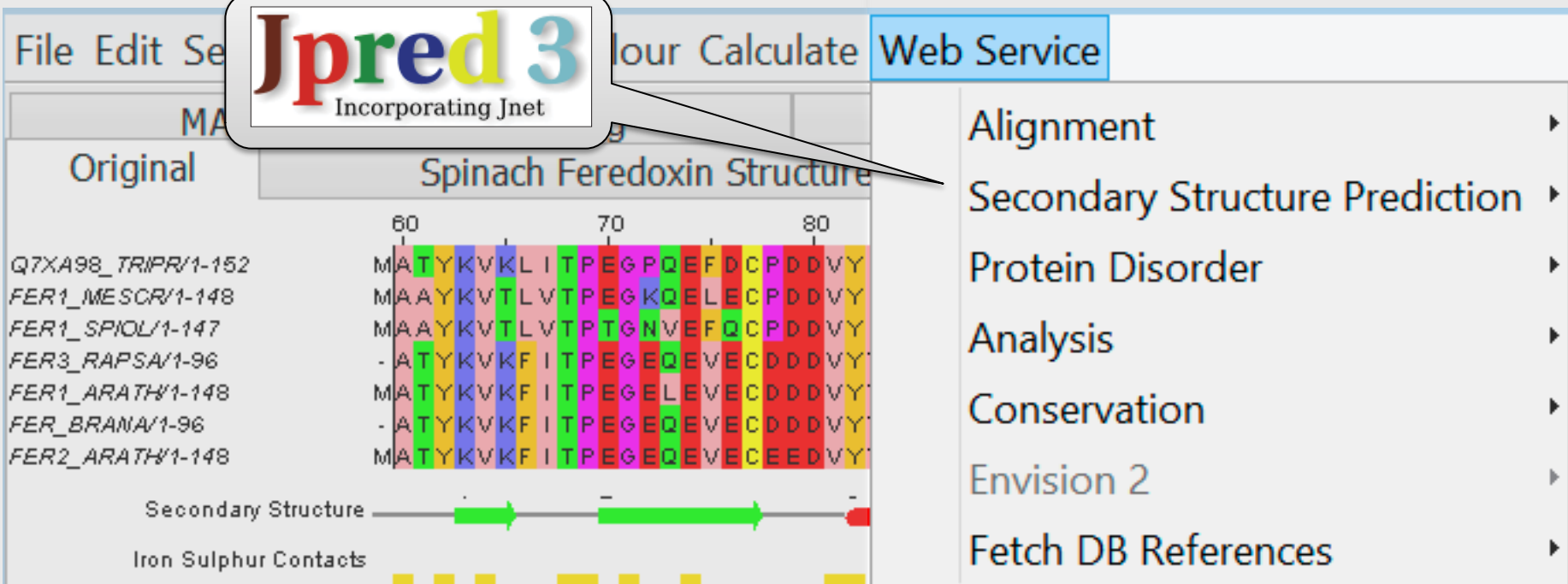
Progress monitored in
job service window

or upload your alignment:

Choose File No file chosen

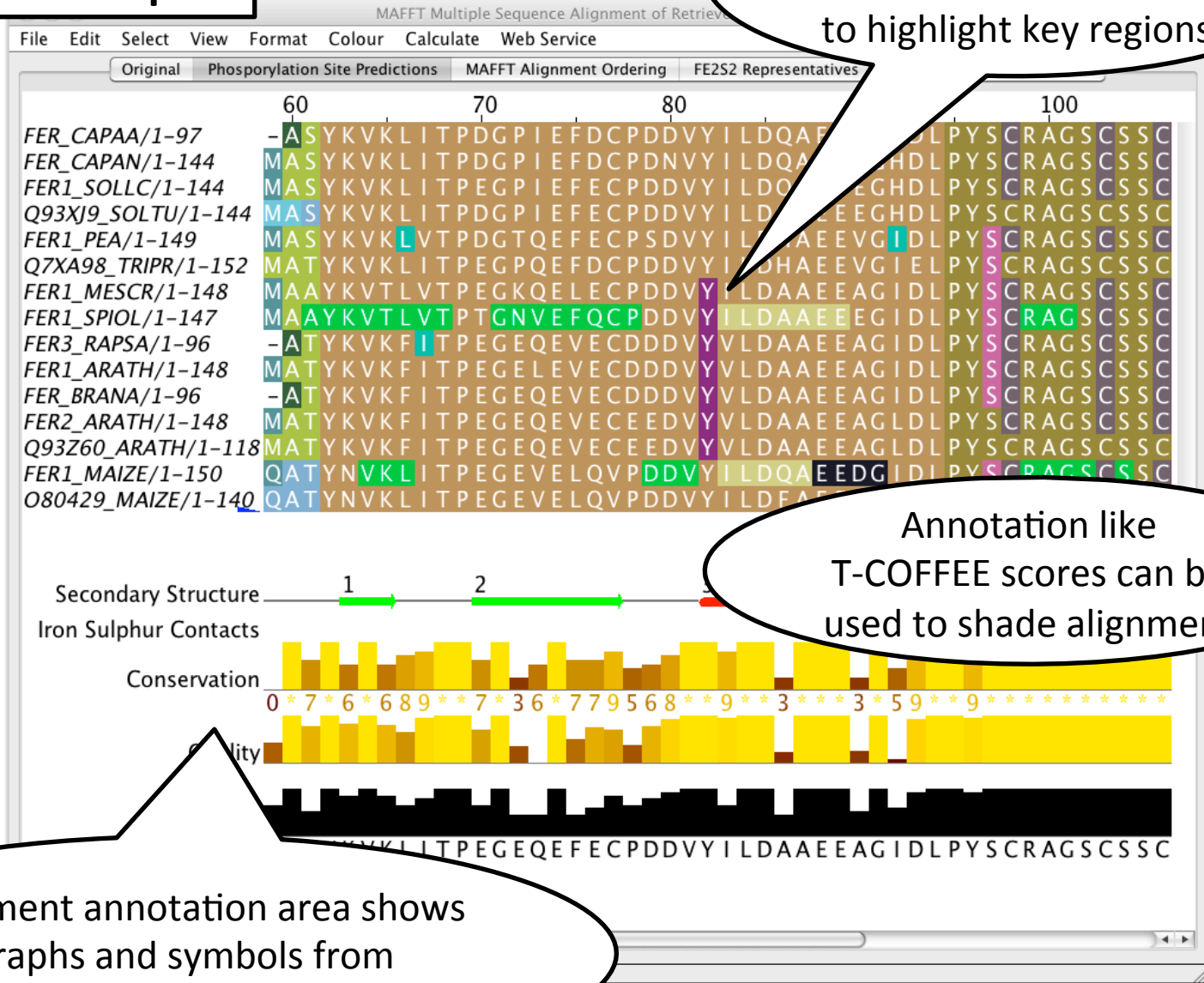
 Provide a list of group sizes:

Example



- Neural network trained on amino acid profiles
 - Predicts **H**elix, **s**h**E**et, or **C**oil 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

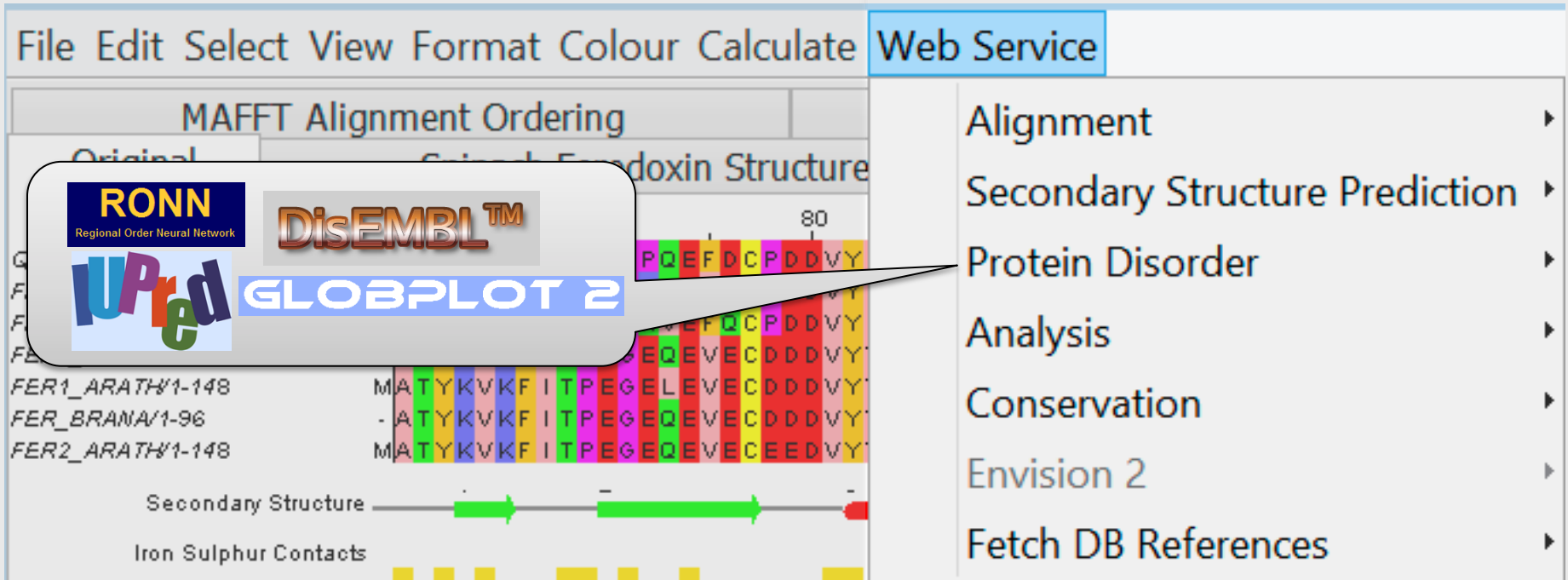
Just to recap...



Sequence features are overlaid on alignment to highlight key regions

Annotation like T-COFFEE scores can be used to shade alignment

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



Protein Disorder prediction

- 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**)

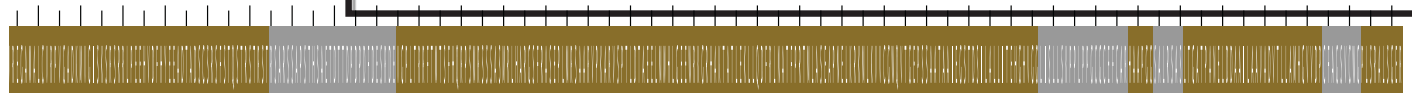
Disorder Predictions from JABAWS

JABAWS
Analysis
Service

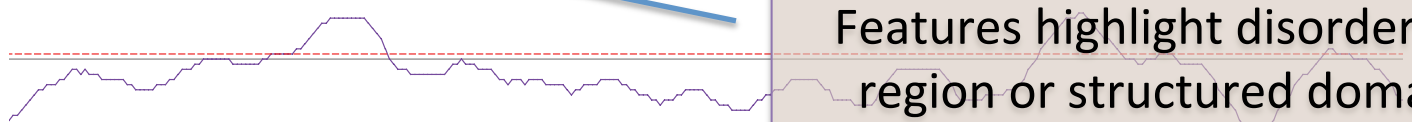
Jalview
JABAWS 2.0
Client

Process results into both
annotation and **features**

☒ DisemblWS	☒ GlobPlotWS	☒ IUPredWS
Feature Type	Colour	Display
Protein Disorder		☒
COILS		☐
REM465		☐
HOTLOOPS		☐
Globular Domain		☒

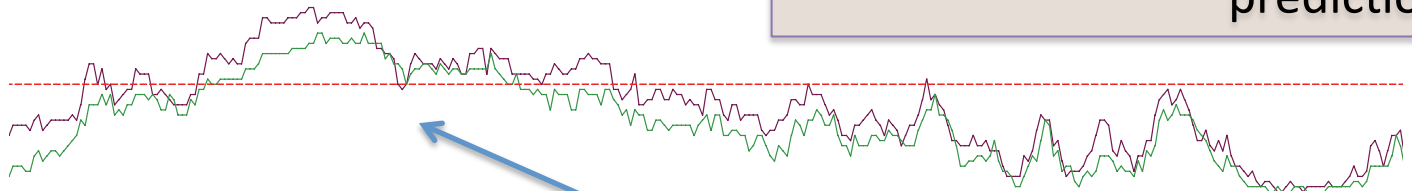


GlobPlotWS (Dydx)



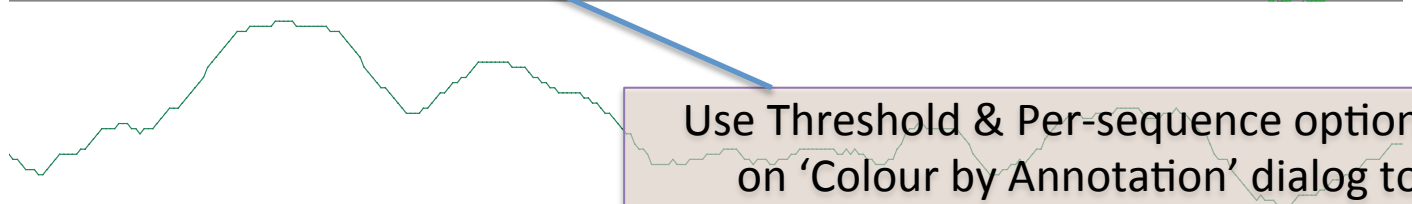
Features highlight disordered
region or structured domain
predictions

IUPredWS (Short)



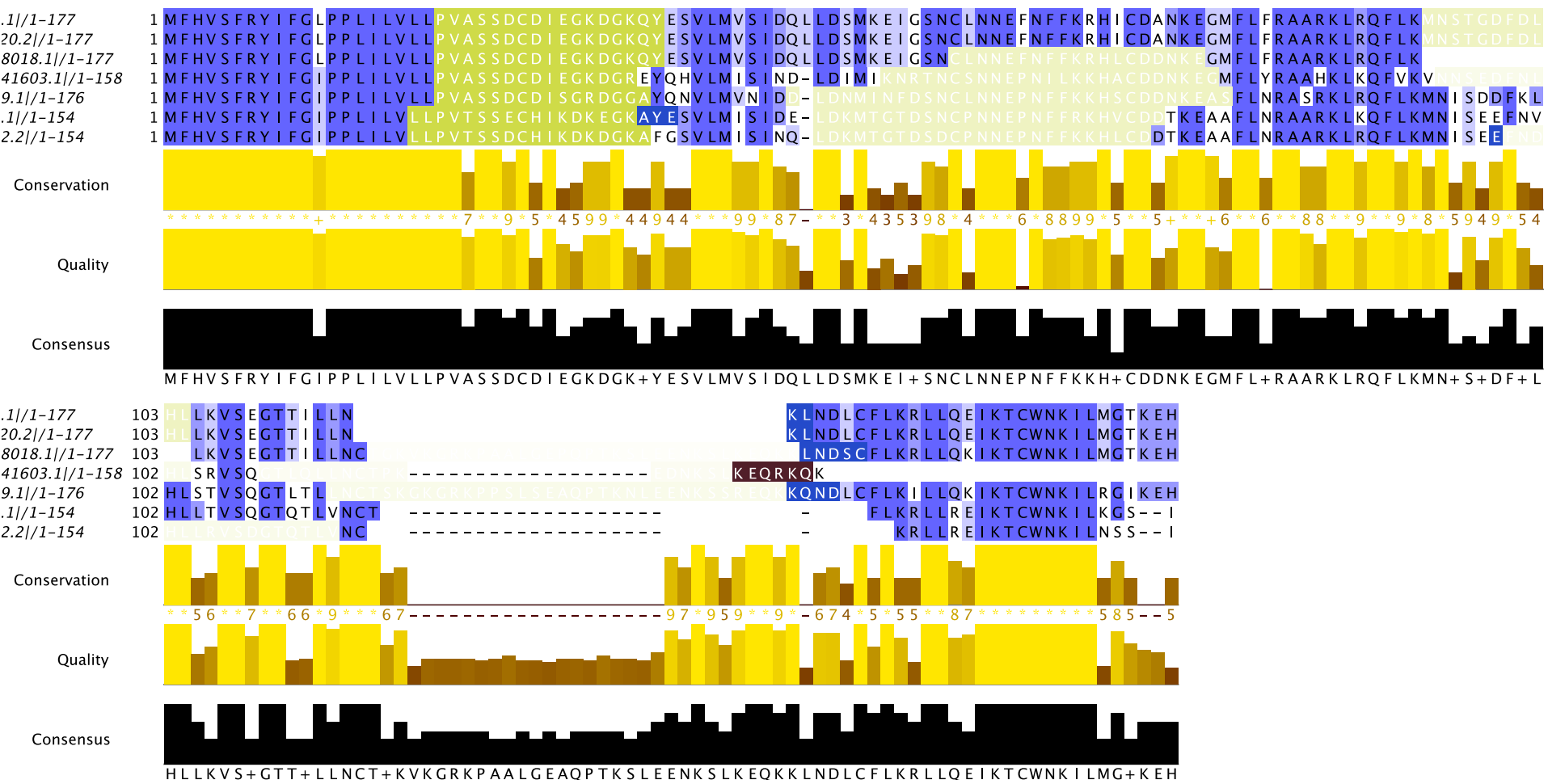
IUPredWS (Long)

JronnWS (JRonn)



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

Disorder in Interleukin 7 Orthologs

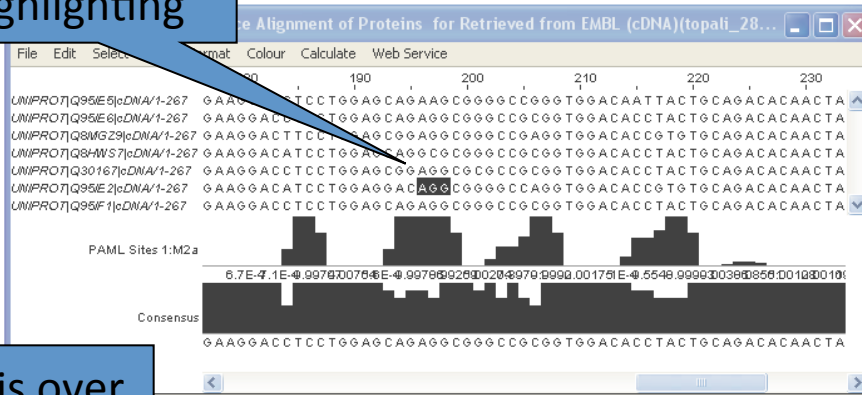


Jalview and Nucleotide data

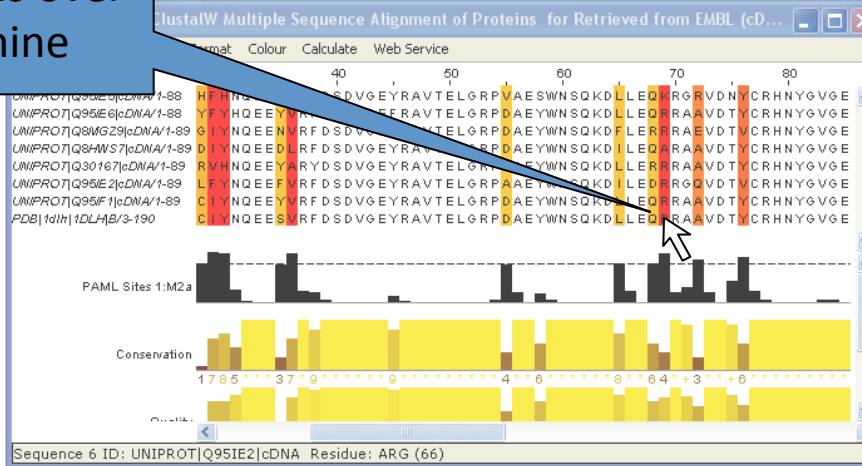
- Basic by current standards
- **Built in cDNA->Amino acid translation**
 - Works with Aligned cDNA
 - Preserves alignment annotation
 - Does **not** backtranslate
- **European nucleotide archive records**
 - Parse cDNA annotation in contigs
- **Display of WUSS or VIENNA RNA secondary structure notation**
 - Stockholm file import
 - LocaRNA Clustal files

Translation of annotated cDNA alignment

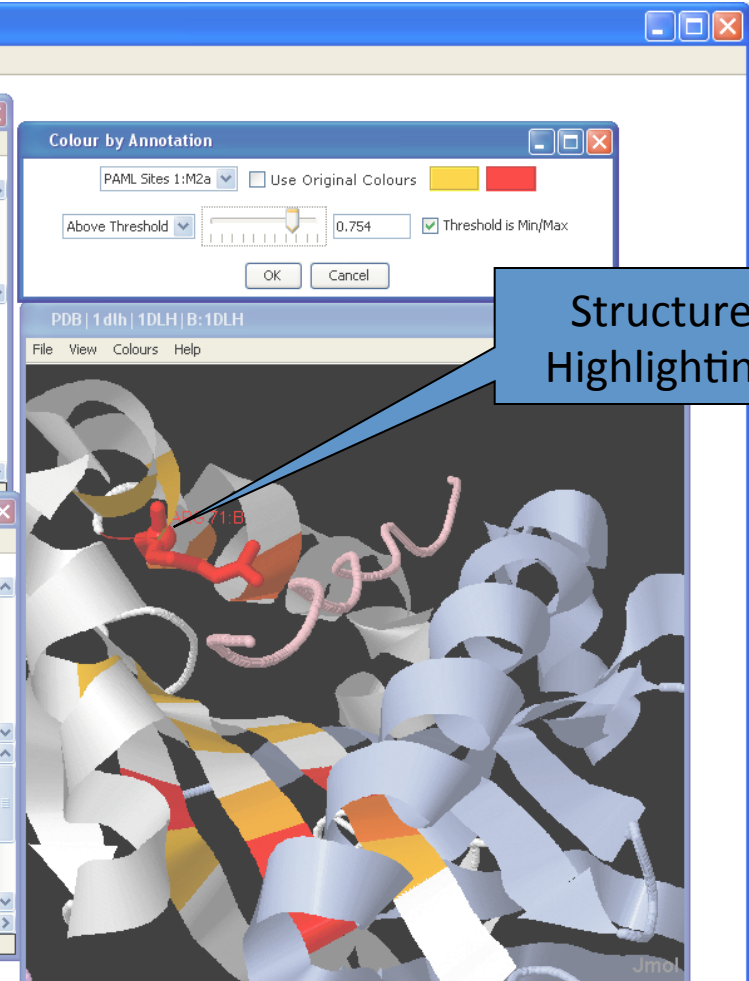
Codon highlighting



Mouse is over Arginine

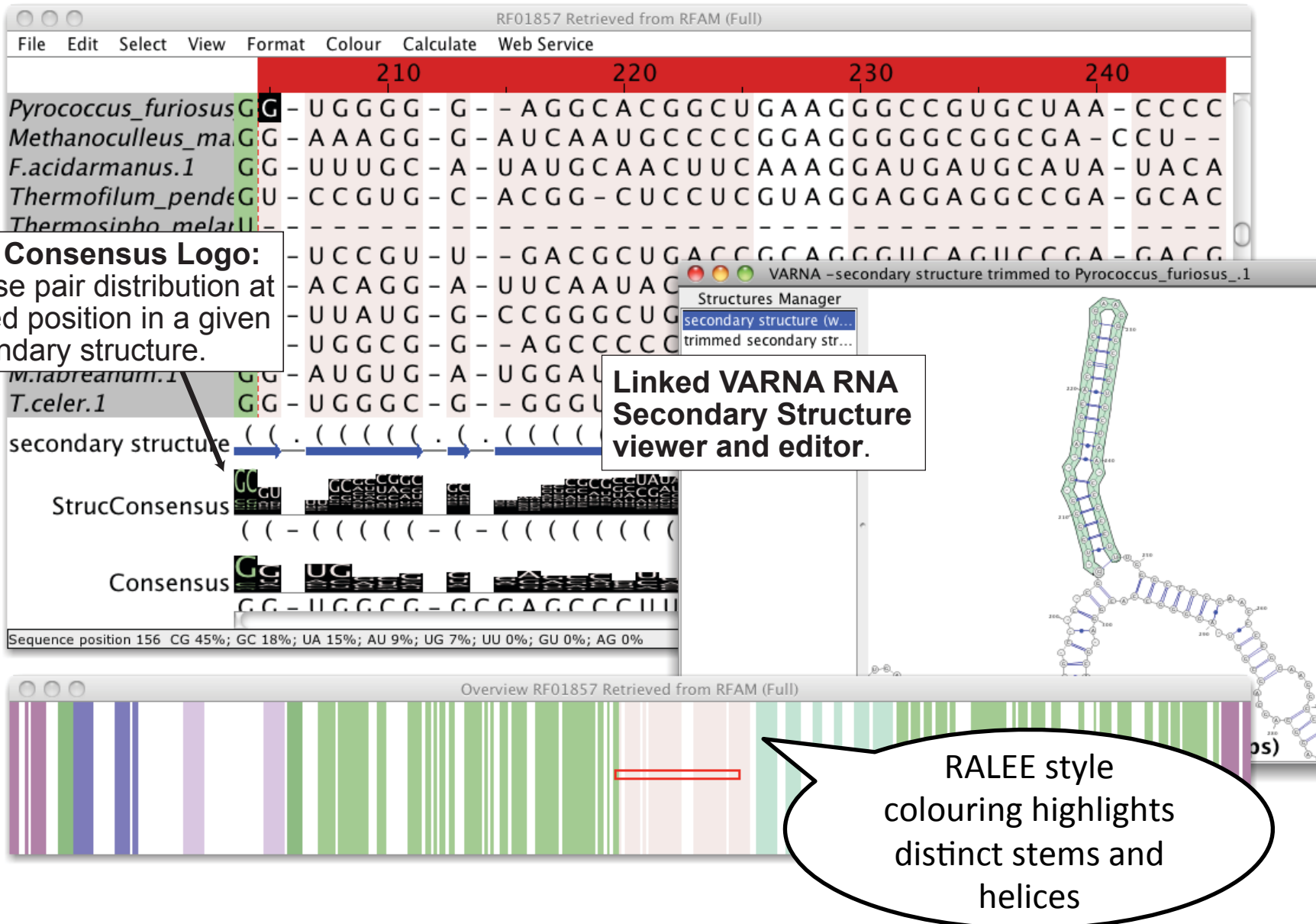


Structure Highlighting



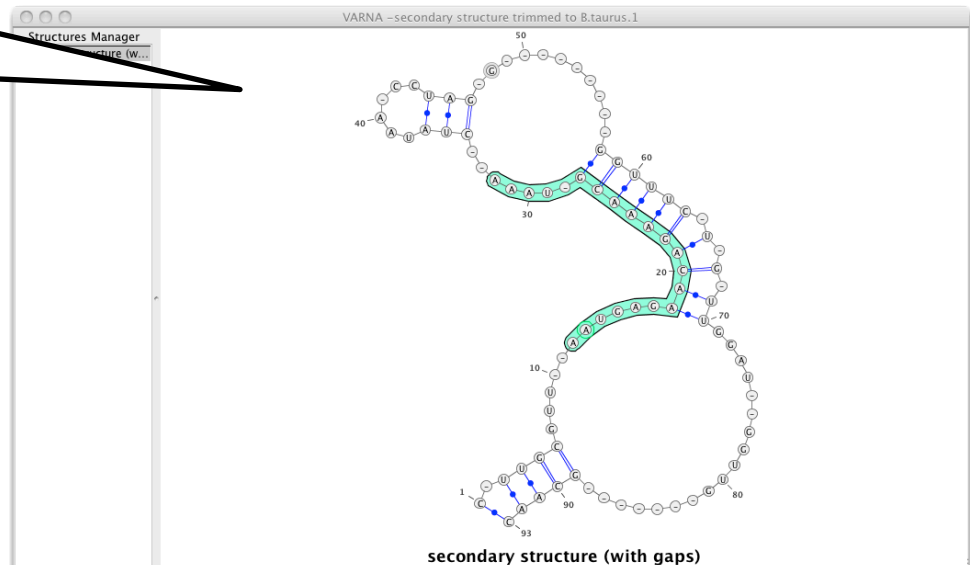
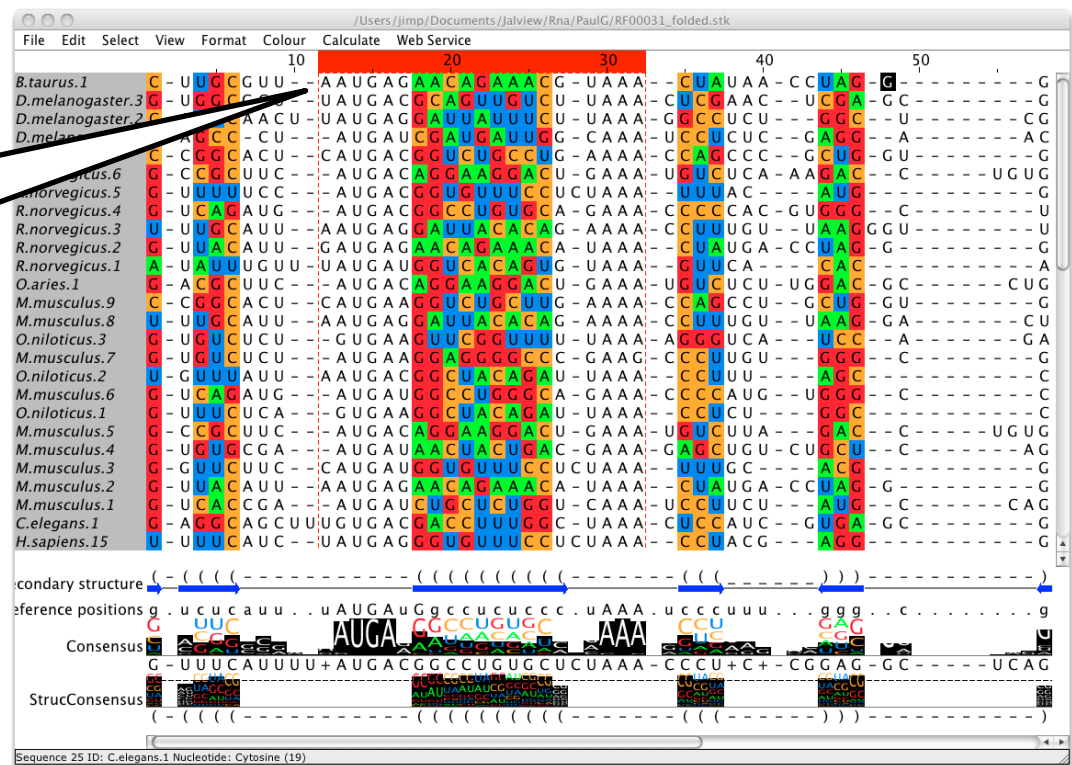
Jalview 2.8 and RNA 2nd-ary Structure

Structure Consensus Logo:
Shows base pair distribution at each paired position in a given RNA secondary structure.



Selections and mouse positions shared between alignment view and VARNA

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

A brief history of Jalview



Jalview
Version 1
1997



Michele Clamp
*Director of Informatics
and Scientific
Applications, Harvard.*

James Cuff
*High Performance
Computing, Harvard.*



Andrew Waterhouse
U. Basel.



Jim
Procter

Steve Searle
*Now at
Sanger, UK*



Jalview
Version 2
2005

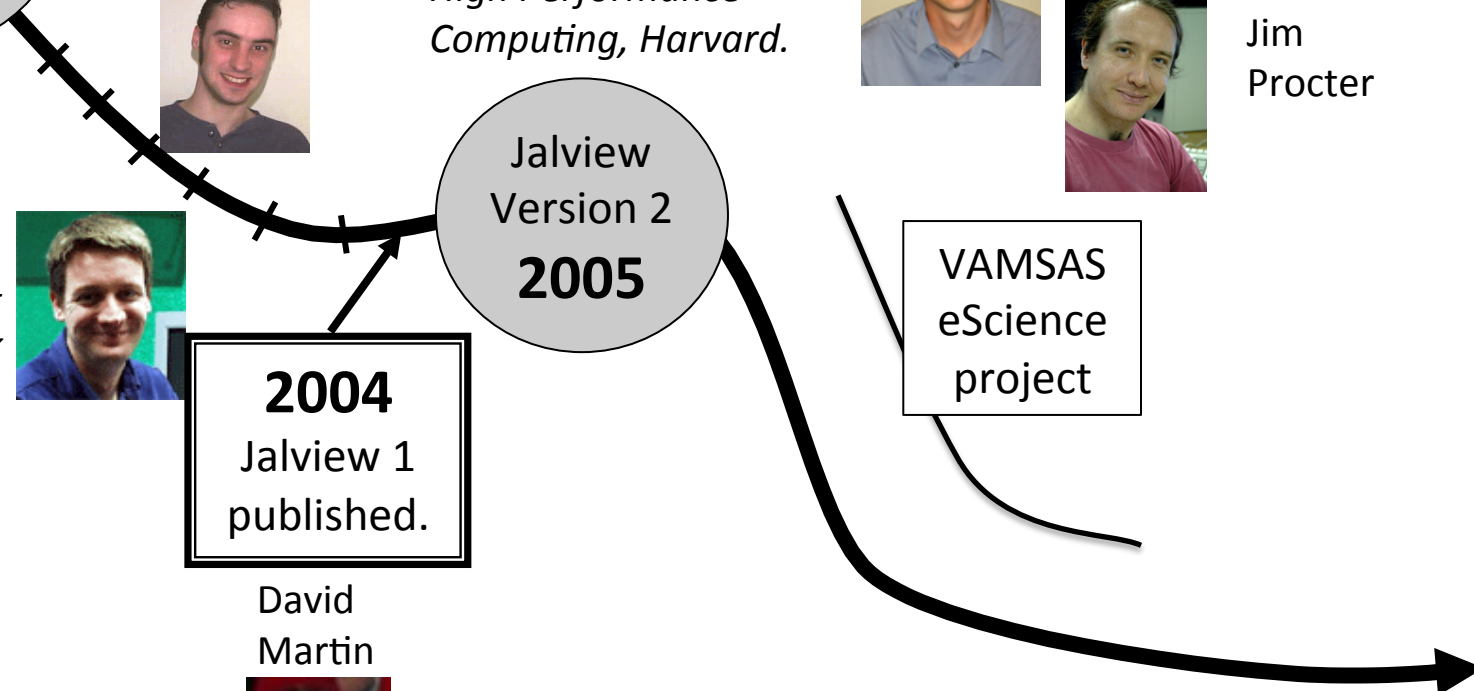
2004

Jalview 1
published.

David
Martin

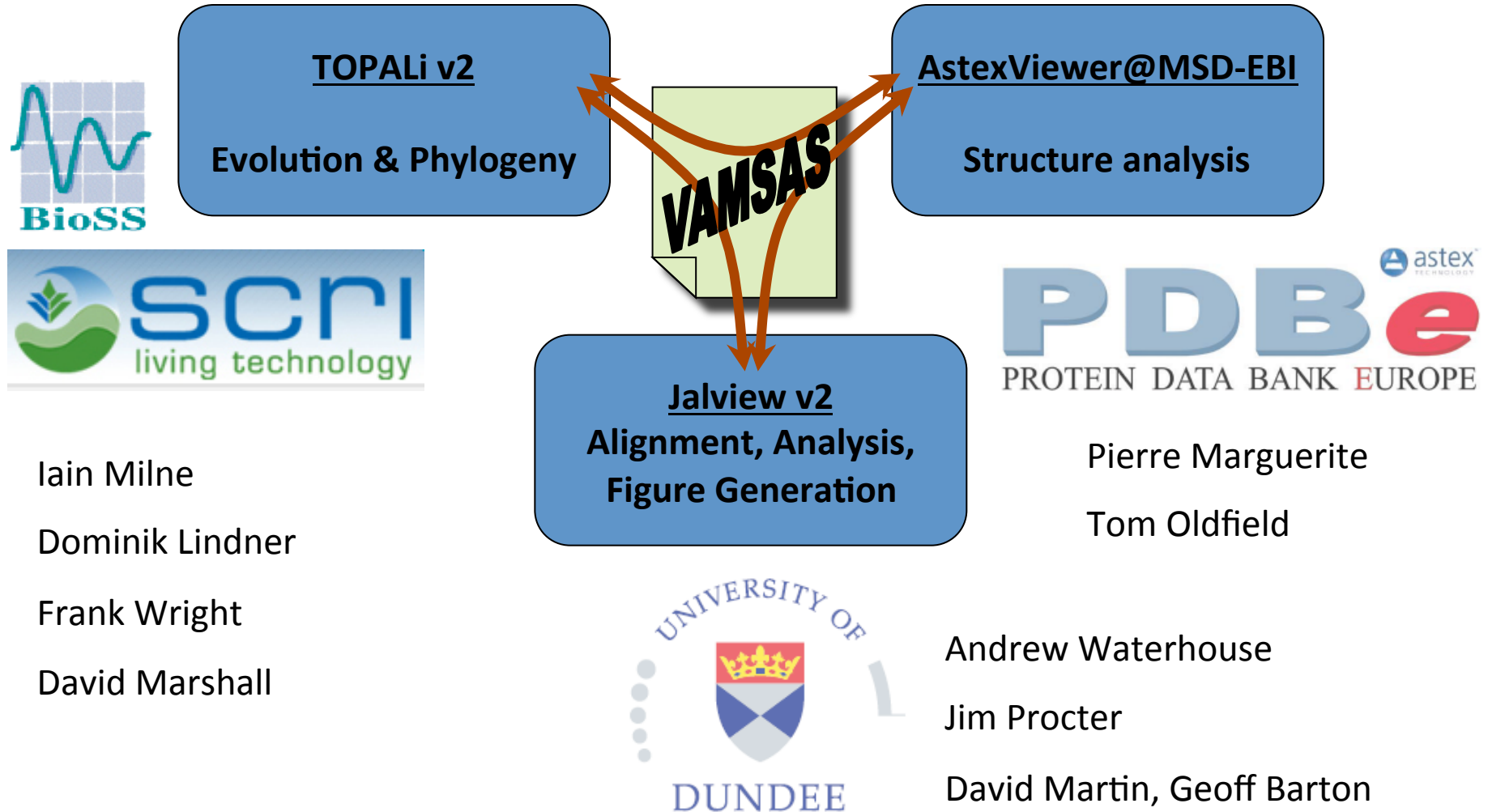


VAMSAS
eScience
project



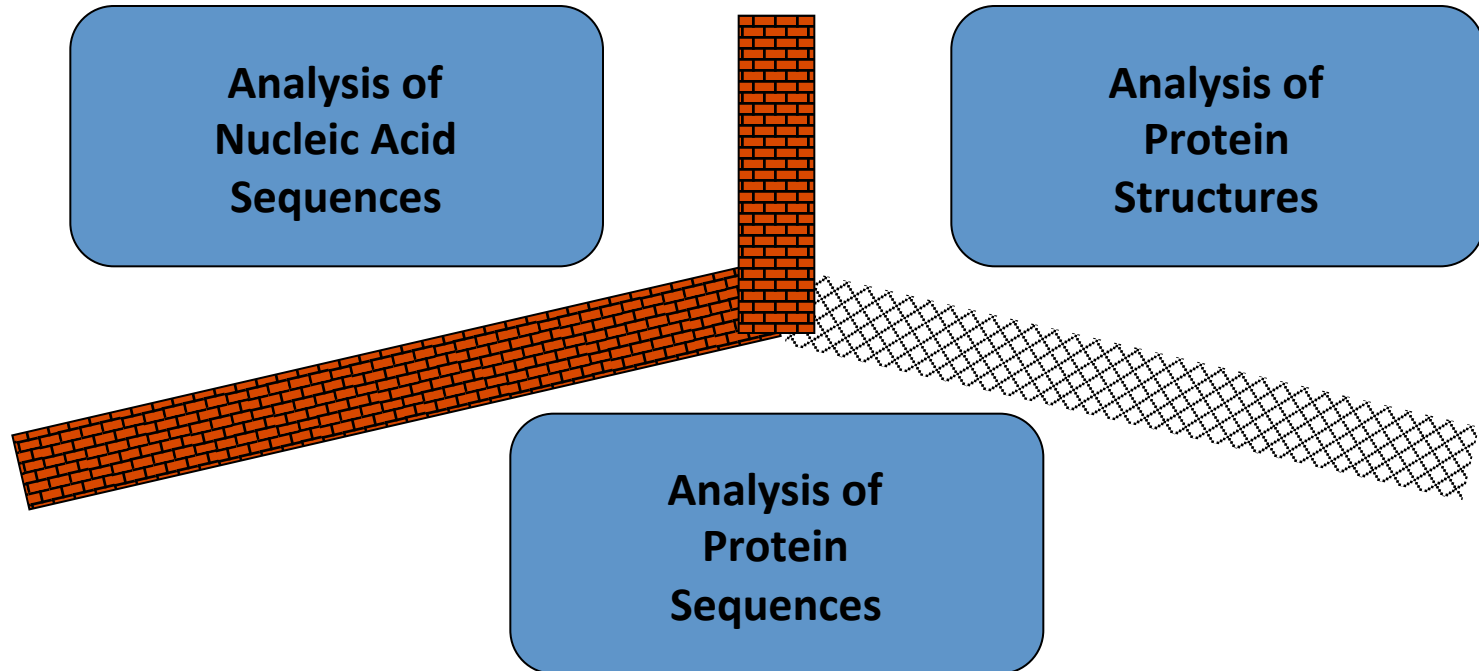
VAMSAS

Visualization and Analysis of Molecular Sequences, Alignments and Structures

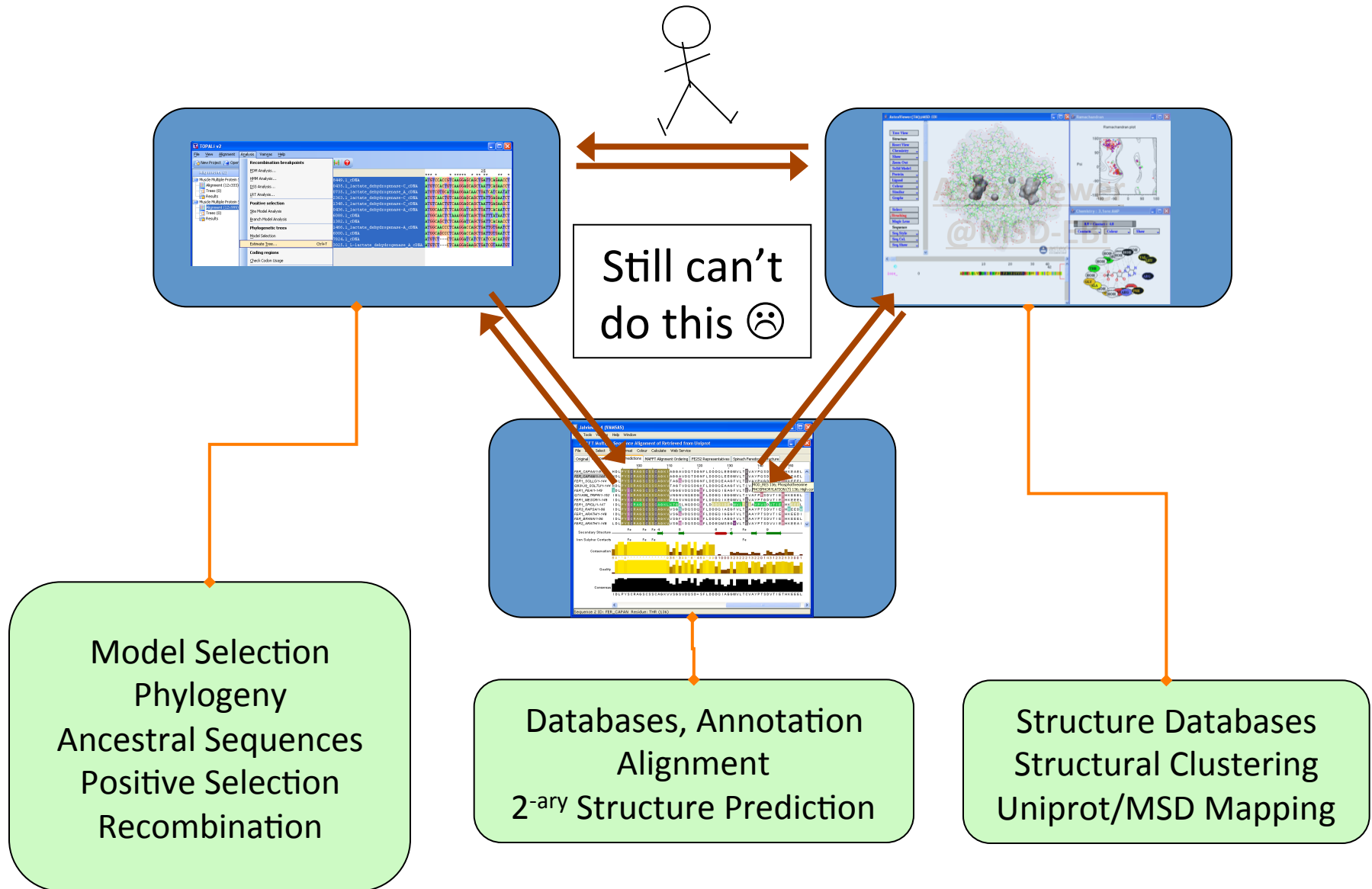


VAMSAS

Visualization and Analysis of Molecular Sequences, Alignments and Structures



Aim: Enable user to move between different VAMSAS Applications



A brief history of Jalview



Jalview
Version 1
1997



Michele Clamp
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James Cuff
*Cycle Computing,
USA.*



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Steve Searle
*Now at
Sanger, UK*



2004
Jalview 1
published.

David
Martin



Jalview
Version 2
2005

Jalview 2 Paper
2009

VAMSAS
eScience
project

2.1

2.2

2.3

2.4

Unsupported graphical tools cause headaches..

User Headaches:

- Can't do what you want:
 - Read/write format 'X'
 - Run my analysis 'Y'
 - Load my 10Gb dataset
- Slow or difficult to use
- Doesn't work properly



Core Developer needed for:

- Staying 'state of the art':
 - New standards
 - New analysis methods
 - New data
- Maintenance
 - Dependencies
 - New OS Versions
 - New hardware
- Hard to do 'research' and maintain software

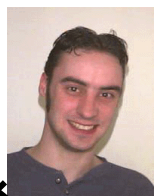
A brief history of Jalview



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Michele Clamp
*Interim Director of
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Jalview 1
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Jalview
Version 2
2005

VAMSAS
eScience
project

2.1

2.2

2.3

2.4

2.5

2.6.1

2.7

2.8

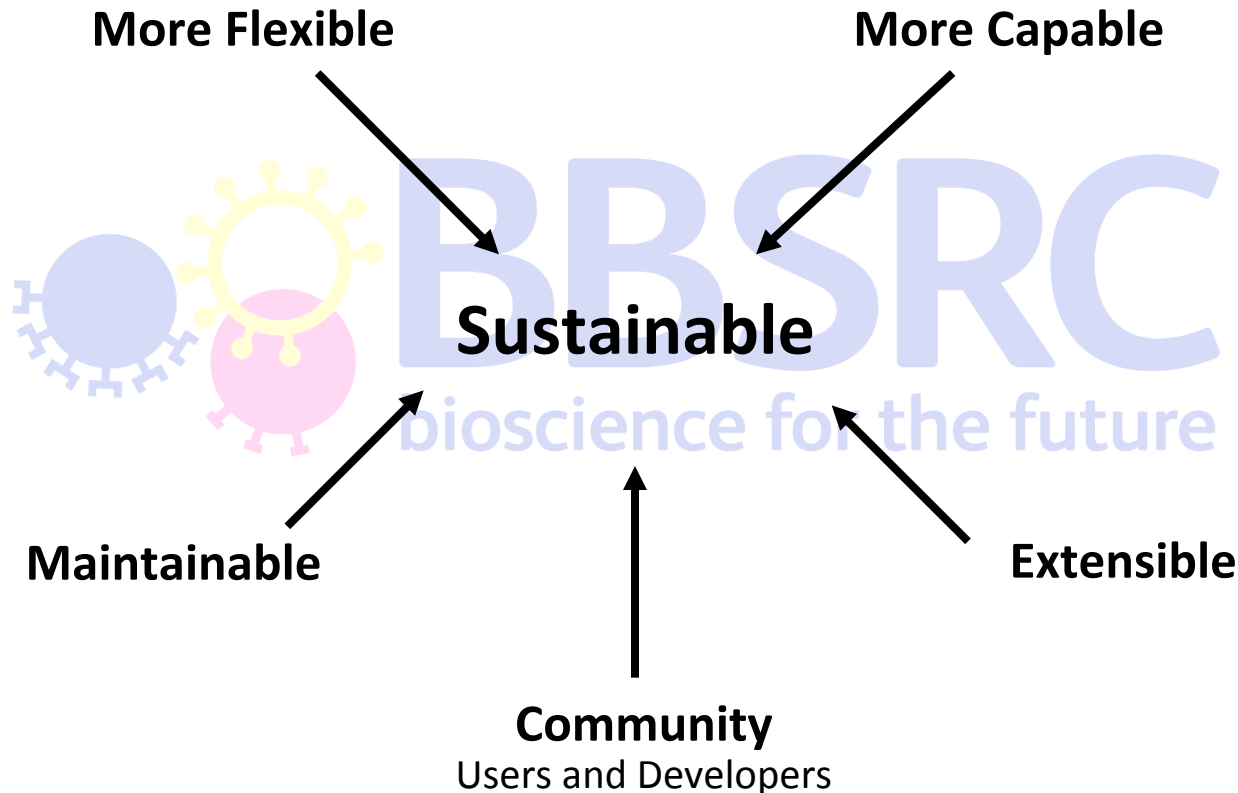
Jalview 2 Paper
2009

New BBSRC Funding
2009-2014

1 Oct 2009

30th Sep 2014

The Jalview 5 Year Plan

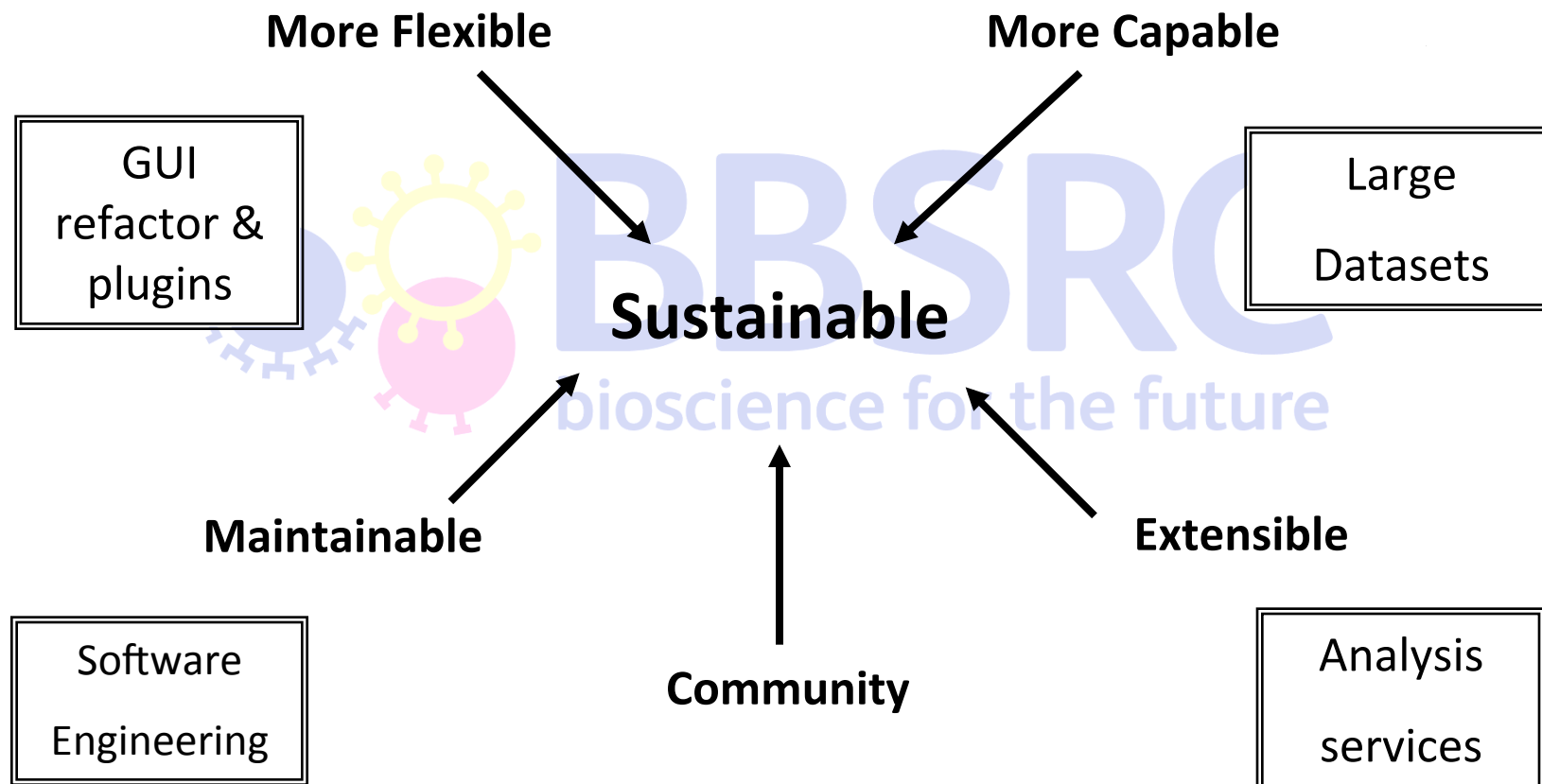


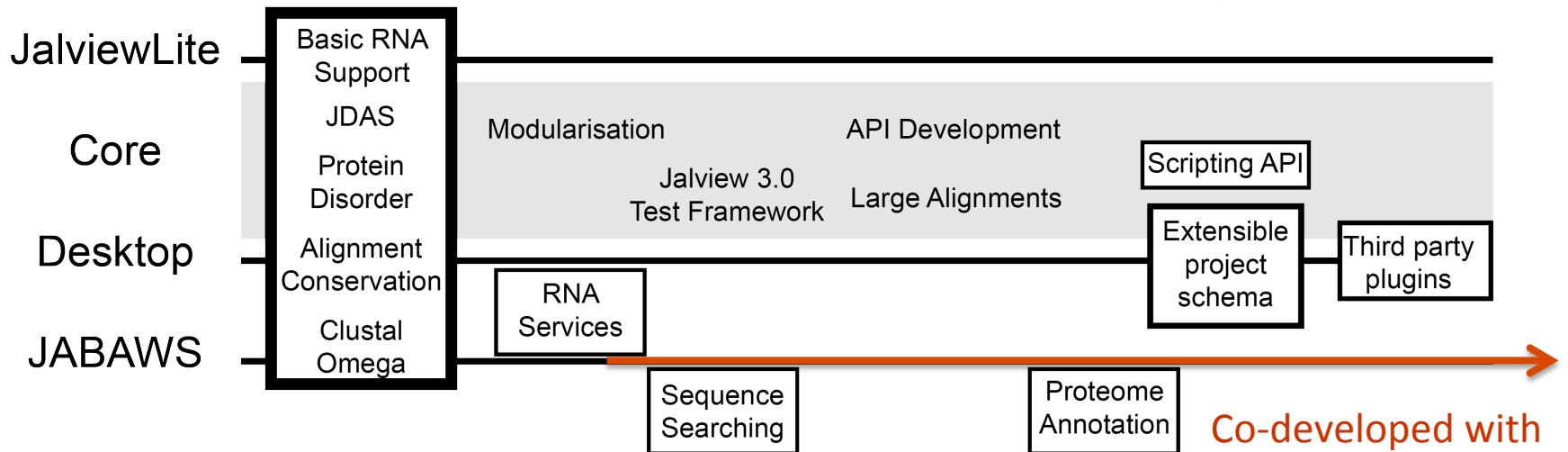
5 Year Tools and Resources Development Fund Grant from the UK
Biotechnology and Biological Sciences Research Council

1 Oct 2009

30th Sep 2014

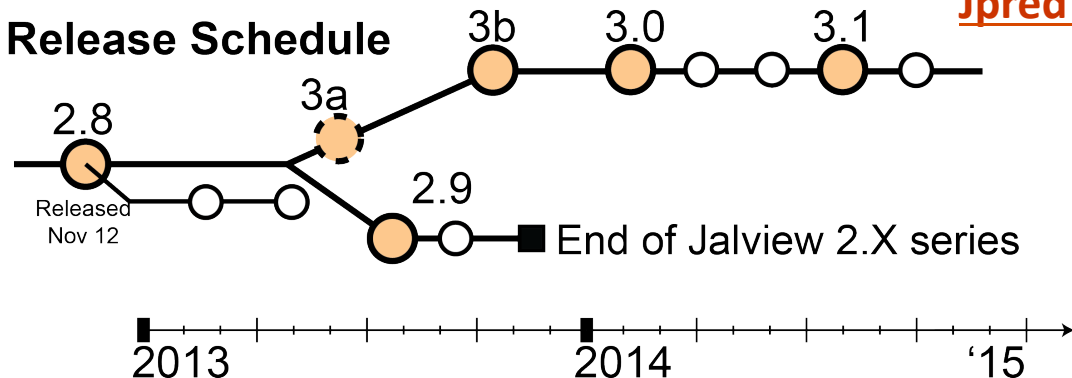
The Jalview 5 Year Plan





Co-developed with
[Sasha Sherstnev](#) on
[Jpred BBSRC BBR](#)

Release Schedule



- Major release
- Minor release
- Alpha or beta release

1 Oct 2009

30th Sep 2014

The Jalview 5 Year Plan

More Flexible

More Capable

Community Outreach

- Website redesign
- Training
 - Users and Developers
- Internationalisation
- True Open Source Development
 - Issue tracker and open repository

GUI
refactor &
plugins

Large
Datasets

Maintain

tensible

Software
Engineering

Analysis
services

Community

Users and Developers



Practical Jalview

guided tutorial and Jalview clinic

Practical Jalview

guided tutorial and Jalview clinic



www.google-melange.com

Google

SUMMER

OF

CODE

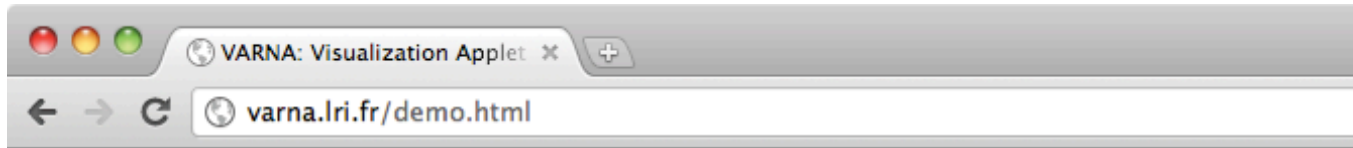
2013



Jan Engelhardt (Uni. Leipzig)



NESCent



VARNA: Visualization Applet for RNA

A Java lightweight component and applet for drawing the RNA secondary structure

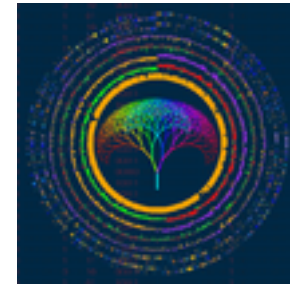
Sequence alignment and secondary structure visualization:

Sequence	U	A	C	C	U	G	U	U	C	A	G	U	U	G	U	A	C	A	-	G	U	A
<i>H.sapiens.11/1-1</i>	U	A	C	C	U	G	U	U	C	A	G	U	U	G	U	A	C	A	-	G	U	A
<i>H.sapiens.10/1-9</i>	U	A	U	C	U	G	U	U	C	A	G	U	U	G	U	A	C	A	-	G	U	A
<i>P.abelii.3</i>	U	A	C	C	U	G	U	U	C	A	G	U	U	G	U	A	C	A	-	G	U	A
<i>P.abelii.2</i>	U	A	C	C	U	G	U	U	C	A	G	U	U	G	U	A	C	A	-	G	U	A
<i>P.abelii.1</i>	U	A	C	C	U	G	U	U	C	A	G	U	U	G	U	A	C	A	-	G	U	A
<i>E.coli</i>	U	A	C	C	U	G	U	U	C	A	G	U	U	G	U	A	C	A	-	G	U	A

Secondary structure diagram (dots and dashes) and sequence alignment (U A C C U G U U C A G U U G U A C A - G U A) are shown below the sequences.



Google Summer of Code 2013 : Why should I participate?



NESCent

Students gain:

- ❖ skills
- ❖ real world experience
- ❖ sample code
- ❖ contacts

Organizations gain:

- ❖ new contributions & contributors
- ❖ global exposure

Google and NESCent Summer of Code 2013

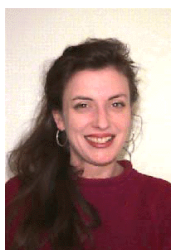
New phylogeny support in Jalview ?

- cDNA/protein editing
 - Display AA translation of cDNA alignment
 - ORF support
- Bacterial genome alignment manipulation
 - New editing
- JABAWS
 - Phylogeny services
 - Extend alignment services to
 - Return guide trees and uncertainty scores
 - Support 'add' and profile alignment



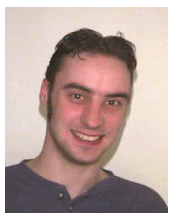
Jalview

www.jalview.org



The Jalview
developers

Michele Clamp
Harvard, USA.



James Cuff
Cycle Computing

Steve Searle
*Sanger,
UK*



Andrew Waterhouse
Basel, Switzerland.



RNA Features

Lauren Lui

UC Santa Cruz, USA.

Jan Engelhardt

Univ. Leipzig, Germany.

Yann Ponty (VARNA)

École Polytechnique, Fr.



T-COFFEE Scores

Paolo di Tomasso

*Notredame Group,
CRG, Spain.*

Geoff Barton (Money)

David Martin (Teaching)

Peter Troshin (JABAWS)

Barry Strachan (logo)

Tom Walsh (Apache)

Ryan Maclaughlan (CSS)

Andrew Millar (Drupal)

All the Jalview users, and ...

