Bioinformatics data is not fun to read.....
## Alignment

<table>
<thead>
<tr>
<th>Accession</th>
<th>Type</th>
<th>Consensus</th>
<th>Quality</th>
<th>Disulfide</th>
<th>Glycosylation</th>
<th>Mature Protein Region</th>
<th>Transmembrane</th>
</tr>
</thead>
<tbody>
<tr>
<td>Q08MGZ9/1</td>
<td>proteolytic</td>
<td>Q</td>
<td>7.6968</td>
<td>0.428</td>
<td>100%</td>
<td>100%</td>
<td>100%</td>
</tr>
<tr>
<td>Q08MGZ9/1</td>
<td>proteolytic</td>
<td>Q</td>
<td>7.8968</td>
<td>0.578673</td>
<td>50.0%</td>
<td>50.0%</td>
<td>50.0%</td>
</tr>
</tbody>
</table>

## Features

- Signal Peptide
- Extramembrane
- Transmembrane
- Polypeptide Domain
- Polypeptide Region
- Glycosylated Residue
- Disulfide Crosslinked Residues

## Structure

<table>
<thead>
<tr>
<th>Atom</th>
<th>Type</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
<th>Charge</th>
</tr>
</thead>
<tbody>
<tr>
<td>ODL</td>
<td>GLU</td>
<td>15.432</td>
<td>67.120</td>
<td>11.132</td>
<td></td>
</tr>
<tr>
<td>ODE1</td>
<td>GLU</td>
<td>16.942</td>
<td>68.587</td>
<td>7.581</td>
<td></td>
</tr>
<tr>
<td>ODE2</td>
<td>GLU</td>
<td>20.412</td>
<td>68.917</td>
<td>8.771</td>
<td></td>
</tr>
</tbody>
</table>

## Tree

- Consensus: 100.0, 100.0, 100.0, 100.0, 42.8
- Consensus: R 100%, F 100%, L 100%, E 0%, H 100%, F 100%, L 100%, E 0%

## Annotation

- MHC class II antigen
- Non-terminal residue
- Mature protein region
- Extramembrane
- Polypeptide domain
- Polypeptide region
- Glycosylated residue
- Disulfide crosslinked residues
Jalview

Java

Standalone or web based

alignment & viewer

and editor

annotation, tree, and structure

Available at

www.jalview.org

www.compbio.dundee.ac.uk
The Jalview Core Team

Geoff Barton
Tochukwu (Charles) Ofoegbu
Kira Mourao
Mungo Carstairs
Suzanne Duce
Jalview & Dundee Protein Resource

supported by
wellcome trust

BBSRC
bioscience for the future
Order of service

9.15 ~ 9.30am  Is everyone sitting comfortably? ...
   Session 1: Getting started: launching, navigation, loading, saving
   Session 2: Selection and editing

10.30 - 11am  Coffee
   Session 3: Colouring, layout, creating figures.
   Session 4: Multiple Alignment (chapter 5)

12 – 1pm  Lunch
   Session 5: Features and annotation (chapter 4)
   Session 6: Alignment analysis (chapter 6)
   Session 7: Working with Structures

3.30 – 4pm  Coffee
   Session 8: Secondary Structure & Disorder Prediction

4.45 - 5pm  Wrapup .. and relax!
Course materials are online

http://www.jalview.org/tutorial/training-materials/2016/Glasgow/

- These slides

- Jalview v2.10.0 Manual (v1.8)

Open the manual NOW!
Latest News
Jalview in 2012 and 2013
Posted On: 12-11-2012

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

Jalview is a free program for multiple sequence
alignment editing, visualisation and analysis. Use
Jalview and edit sequence alignment files and
analyse them by principal component analysis
(PCA) plots and explore molecular structure
and annotation.

Jalview training news and course dates

Jalview Community

Jalview Development and release history

Installation packages and source

Help and documentation

http://www.jalview.org
Where to Find Help?

Help
- Getting Started
- FAQ
- Discussion Mailing List
- Other Resources

Community
- News Mailing List
- Discussion Mailing List
- Links
- Community News

Development
- Jalview Bug Tracker
- Development Version
- Jalview Git Web
- Version Archive
- Release History
- Development News

Training
- Training Courses
- Training Videos
- Training News
- Jalview & JABA Slides

Jalview
The Jalview Team based at School of Life Sciences, University of Dundee, UK

487 views 1 year ago

Jalview Online Training YouTube Channel is a free bioinformatics educational course suitable for Undergraduate and PhD students. Playlists include (a) Getting Started; (b) Selecting and Editing Sequences; (c) Colour, Appearance and Figure Generation; (d) Jalview Dundee.

This video features Dr Suzanne Duce, Dr Jim Procter, Mr Mungo Carstairs, Mr Charles Tochukwu Ofoegbu, Dr Alexey Drozdetskiy, Mr Dmitry Finkelbergs and Pri...
Printed Manual & Online Videos

- Basics
- Selecting and Editing Sequences
- Colouring Sequences and Figure Generation
- Annotation and Features
- Multiple Sequence Alignment
- Analysis of Alignments
- Working with 3D structures
- Protein sequence analysis and structure prediction
- DNA and RNA Sequences
- Webservices

- Getting started
- Selecting & Editing
- Colour, Appearance and Figure Generation
- Analysis and annotation

Not covered today – some exercises out of date
Jalview comes in two flavours

The Jalview Desktop

Analysis Services

Biological Data Services

The JalviewLite Applet

Javascript API

import from web

applet parameters

Alignment And Annotation

Bioinformatics Web Server

Launch Jalview Applet

Launch Jalview Desktop
The web was where Jalview started

http://pfam.xfam.org/family/bromodomain#tabview=tab3
Ex 1 – starting
The Jalview Desktop

Webstart links for different memory settings


7GB  http://www.jalview.org/services/launchApp?jvm-max-heap=7G&version=Release

Launching the jalview desktop

Version: 2.10.0
Last Updated: 13 October 2016

Authors: Jim Procter, Mungo Carstairs, Tochukwu 'Charles' Ofoegbu, Andrew Waterhouse, Jan Engelhardt, Lauren Lui, Anne Menard, Daniel Barton, Natasha Sherstnev, David Roldan-Martinez, 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/faq and/or join the jalview-discuss@jalview.org mailing list

If you use Jalview, please cite:
Jalview Version 2 - a multiple sequence alignment editor and analysis workbench
Bioinformatics doi: 10.1093/bioinformatics/btp033
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)
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.
Anatomy of Jalview: Figure 1.7
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

An online video about using jalview is available at http://www.jalview.org/Help/Getting-Started
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

An online video about using jalview is available at http://www.jalview.org/Help/Getting-Started
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?
END of Session 1: Getting Started

- Launching the Jalview Desktop
- Navigation
- Getting data into Jalview
- Two modes:- Normal and Cursor
- Saving alignments and projects
Session 2: Selecting and Editing Sequences

- Selecting rows, column and groups
- Reordering sequences
- Hiding columns and rows
- Editing in Normal mode and Cursor mode
Ex 5

selecting regions & making groups

• Task
  – Get used to marking parts of the alignment with the mouse and keyboard
  – Learn how to create and remove groups

An online video about selection and creating groups is available at
http://www.jalview.org/training/Training-Videos
Ex 5
selecting regions & making groups

• Task
  – Get used to marking parts of the alignment with the mouse and keyboard
  – Learn how to create and remove groups

Question:
• What happens if you press the up/down arrow keys?
Ex 6
Reordering the alignment

• Task
  – Get used to selecting and reordering sequences

Question:
• What’s the quickest way to move the bottom-most sequence to the top of the alignment?
• What other ways can you reorder sequences?
Ex 7
hiding & showing

Task

• Learn about hiding columns and rows in the alignment

An online video about selection and creating groups is available at
http://www.jalview.org/training/Training-Videos
Ex 7
hiding & showing

Task
• Learn about hiding columns and rows in the alignment

Question:
• Why would you create representative sequences?
Alignment editing

• Exercise 8 and 9 let you practice mouse and keyboard based editing techniques

• Try them over the weekend!
Alignment editing modes

[F2] (PC)
toggle between Normal and Cursor Mode

[F2] & Fn (Mac)
toggle between Normal and Cursor Mode
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.
<table>
<thead>
<tr>
<th></th>
<th>Original</th>
<th>Phosp</th>
</tr>
</thead>
<tbody>
<tr>
<td>/1-148</td>
<td>MAST----A</td>
<td></td>
</tr>
<tr>
<td>/1-150</td>
<td>MATVLGSPPR</td>
<td></td>
</tr>
<tr>
<td>/1-148</td>
<td>MAAT----TAA</td>
<td></td>
</tr>
<tr>
<td>-149</td>
<td>MATT----PA</td>
<td></td>
</tr>
<tr>
<td>/1-144</td>
<td>MA----S</td>
<td></td>
</tr>
</tbody>
</table>
F2 enables/disables keyboard mode

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

F2 enables/disables keyboard mode

Windows 7 Users:
Group Insert - use Shift+Space
(not CTRL+Space)
Locked Editing

- Allows you to insert gaps without affecting downstream alignment
END of Session 2: Selecting and Editing Sequences

- Selecting rows, column and groups
- Reordering sequences
- Hiding columns and rows
- Editing in Normal mode and Cursor mode
Session 3: Colouring, layout & figures

- Colouring sequences and alignments
- Changing layout of the alignment
- Creating figures
Ex 10: Colouring

• Tasks
  – Learn how to colour all, or part of the alignment by
    • Amino acid property
    • Alignment conservation

• Questions
  – Why is colouring the alignment useful?
  – How would you highlight acidic residues in your alignment?
Ex 10 : Colouring

• Tasks
  – Learn how to colour all, or part of the alignment by
    • Amino acid property
    • Alignment conservation

• 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, SVG 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?
Out of date figures…
Look carefully at the menus!
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, SVG 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?
  – What happens when you drag an exported HTML file back on to Jalview?
END of Session 3: Colouring, layout & figures

- Colouring sequences and alignments
- Changing layout of the alignment
- Making figures
Session 4: Multiple Sequence Alignment

- Performing alignments with Jalview
- Understanding how hidden regions affect alignment
- Changing alignment parameter settings

JABAWS 2 In Preparation.

Native JABAWS installs on a range of platforms

JABAWS Virtual Appliance for your private use.

JABAWS Amazon Machine Image on EC2

powered by

Jalview Web Service GUI

JABAWS Java Client


JABAWS 2 In Preparation.
Clustal Omega quick alignment of millions of sequences

Assorted protein disorder predictors

Protein conservation calculations

JABAWS 2 services in Jalview 2.8
Jalview’s Alignment Methods

• **Multiple alignment**
  – Provided as Web Services

• **Pairwise alignment**
  – Needleman and Wunsch
Why do we provide so many?

• Different purposes
  – Large alignments
  – Difficult sequence families
  – Special score models
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**, also employ sampling strategies to speed up tree building & refinement.
Why do we provide so many?

- Different purposes
  - Large alignments
  - Difficult sequence families
  - Special score models
- Reproducibility
  - Older methods still widely used
- Special features
Multiple Sequence Alignment
exercise 16 (Section 5.2)

• Tasks
  – Align sequences using different methods
  – Explore how hidden regions affect alignment jobs.
Multiple Sequence Alignment
exercise 16 (Section 5.2)

• Tasks
  – Align sequences using different methods
  – 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?
Realignment with ClustalW & ClustalO

1. Import a good alignment
   - E.g. a PFAM seed

2. Add more sequences
   - ClustalW
     - Preserves original alignment
     - Align new sequences to profile
   - ClustalO
     - Builds profile
     - Aligns **ALL** sequences to profile
Custom Analysis Parameters

Browse or edit to change name of set

Buttons appear to create, update, rename or delete user settings.

text box to add notes for the parameter set

Parameters contains more complex settings

Start job with current settings or cancel.

Tooltips give brief description and link (right click) to further info
Modifying 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?
End of Session 4:
Multiple Sequence Alignment

- Performing alignments with Jalview
- Understanding how hidden regions affect alignment
- Changing alignment parameter settings
Session 5: Features, Annotation, Databases

- Understand the difference between Features and Annotation
- Learn where features & annotation come from
- Customise feature display
- Use feature and annotation to query the alignment
Features are annotations on sequences.

- Manually created
- Calculated from alignment

Annotation area shows graphs and symbols.
Select by annotation
Sequence Features have:
Name, Description, Group
Adding Features Manually
Create New Feature...

Name: Binding site
Group: Jalview
Colour: Purple
Description: Deduced by homology
Sequence Features are visualised over the alignment
Customising Feature Display

View => Feature Settings…

- Drag features to reorder on alignment
  – Or make transparent
- Change colour
- Enable/disable by name and group
Customising Feature Display

Right-click on feature => Popup menu

Select or hide columns
Customising Feature Display

Graduated Colour Scheme
Sources of sequence features

• Sequence databases
• 3D Structure associations
• GFF2/3 (*Generalised Feature Format*)
• Jalview format feature files
• Certain ‘rich’ alignment text file formats
  – Stockholm
  – AMSA
• Manual input of features in Jalview
Sources of sequence features

• Sequence databases
• 3D Structure associations
• GFF2/3 (Generalised Feature Format)
• Jalview format feature files
  – Like GFF
  – can create GFF in Excel
  – Allows scores to be added
Annotated Contigs, cDNA and products

3D Structures provide Features & Annotation

Annotated Protein Domain Alignments

Annotated Protein Sequences

Annotated RNA Domain Alignments
Retrieve from database

Match sequence to database record
Ensembl – new in Jalview 2.10

• Principal source for
  – Reference genomes
  – Transcripts
  – Protein products

• Sequence variants
Retrieve Ensembl ENSG0000016779

Transcripts shown aligned to gene locus

Calculate=> Cross-references => Uniprot

CDS/Protein split frame shows isoforms and variant sites

Variants on genomic reference propagated to product
Retrieve Ensembl ENSG0000016779

Transcripts shown aligned to gene locus

‘Predefined’ ordering and colours for features

Calculate => Cross-references => Uniprot

CDS/Protein split frame shows isoforms and variant sites

Product alignment includes gaps for misaligned codons

Variants on genomic reference propagated to product
‘Split Frame’ cDNA & Protein MSAs

Opened with any linked cDNA/Protein data
e.g.
- ENA records
- Flat file
- cDNA translation

cDNA/Protein Alignment Reconstruction:
- Gaps inserted according to ‘reference alignment’

Layout and display are configurable.
‘Split Frame’ cDNA & Protein MSAs

Linked alignments share:
- Selections
- Gap editing
- Multiple Views
- Tree sub-groups

Allow new Capabilities
- Codon conservation
End of Session 5: Features and Annotation

- Understand the difference between Features and Annotation
- learn where features & annotation come from
- Customise feature display
- Use feature and annotation to query the alignment
- CDS/Protein split-view
- Ensembl
- ‘Show Cross-references’
Alignment Analysis

Using jalview to analyse the relationships between aligned sequences.
Session 6: (Chapter 6)
PCA, Trees & subfamily analysis

- 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, good for understanding alignment structure
  – Neighbour joining
    • Slower than UPGMA
    • Useful for a first approximation for evolutionary analysis
      – 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 Trees
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 Trees
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
Exercise 20

• “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

Exercise 20

• “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 ?
  – How can you navigate the sub-groups of a large alignment ?
Sub-groups and Sub-group Annotation
Exercise 22

• Task
  – Use the group consensus sequence logos to more easily compare tree subgroups
  – Use ‘Make groups for selection’ to subdivide groups by specific mutation
End of Session 6: (Chapter 6)
PCA, Trees & subfamily analysis

- Principal component analysis
- Phylogenetic trees
- Redundancy removal
- Tree based conservation analysis
- Subdividing alignment by mutation
Session 7: 3D structures in Jalview

Learning objective:
- Viewers supported by Jalview
- Configuring default structure viewer
- Methods of importing structures in Jalview
- Structure to Sequence mapping and methods
- Structure coloring and annotations
- Superimposing structures with MSAs
Associating structures with sequences

- Structures in the PDB database
  - Auto-discovered using database references
  - Provide PDB ID (and chain) for sequence

- Local PDB file
  - Drag and drop to match files to sequences by ID
  - Attach PDB file to sequence manually
Secondary structure annotation tracks from 3D Structure

• Jalview ‘Structure’ preferences tab

Enable/Disable Jmol
DSSP

RNA structures processed with web service (slow!)

Automatically add tracks to alignment
3D Structure Visualization in the Jalview Desktop

Integrated with Jalview

External program called by Jalview

jmol.sourceforge.net

www.rbvi.ucsf.edu
Configure Jalview and Chimera

- Jalview ‘Structure’ preferences tab

  - Toggle between structure viewers
  - Set path to C:\Programs \Chimera\bin\chimera
Which viewer to use for the exercises?

- Jmol is friendly for people new to structure.
- If you know Chimera and have it installed, use it!
Protein Structures in Jalview
Exercise 23

• Task
  – Discover PDB structures for ferredoxin sequence(s)
  – Save and load structures and manipulate colouring
Protein Structures in Jalview
Exercise 23

• Task
  – Discover PDB structures for ferredoxin sequence(s)
  – Save and load structures and manipulate colouring

• Questions
  – What happens if there are lots of structures?
  – What annotation & features come from structure?
Choosing a structure to view

- Auto-select best structure by criteria
- View structure(s) after selection
- Toggle to inverse auto-selected option
- Add or remove summary columns
- Auto-selected structure
Structure unavailable?

Switch manual association method
Viewing sequence-structure mapping

Alignment Sequence

Mapping summary

Mappings

Structure Sequence

Percentage ID = 98.97
Exercise 25 Superposing Structures using Alignments

• Task
  – Align structures using the ferredoxin alignment
  – Experiment with views to control what part of the alignment is used to superimpose the structures
many structures can be shown in a single view

Structures can be Superimposed using the visible region of alignment
Exercise 25 Superposing Structures using Alignments

• Task
  – Align structures using the ferredoxin alignment
  – Experiment with views to control what part of the alignment is used to superimpose the structures
Exercise 25 Superposing Structures using Alignments

• 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?
Colouring structures using many multiple alignments

Exercise 26 – Homework!
End of Session 7: 3D structures in Jalview

Learning objective:

- Viewers supported by Jalview
- Configuring default structure viewer
- Methods of importing structures in Jalview
- Structure to Sequence mapping and methods
- Structure coloring and annotations
- Superimposing structures with MSAs
SECONDARY STRUCTURE PREDICTION

RNAAlFold
Not today!

PROTEIN DISORDER PREDICTION
http://www.compbio.dundee.ac.uk/jpred

Jpred 4
Incorporating Jnet

A Protein Secondary Structure Prediction Server

Input sequence

MQVWPIEgilLKFTLYLPRLKGEYLLRSKWKWPLELSKEFSGVFYRENHRSPGYYDGYW
TMWKLPMFGCETATQLKEELAKKAYPDAFVRIGFDNVRQVQLSFIAYKPPGC

Advanced options (click to show/hide)

Make Prediction  Reset Form

More citations: link.
Protein Secondary Structure Prediction
Section 8.1

- 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 27

• Tasks
  – Perform a variety of Jpred4 predictions
    • Note the effect of hidden regions
    • Learn about sequence associated annotation
    • Learn about reference sequence views

• Questions
  – …
Exercise 27

• Tasks
  – Perform a variety of Jpred4 predictions
    • Note the effect of hidden regions
    • Learn about sequence associated annotation
    • Learn about reference sequence views

• 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?
Exercise 28 – Disorder predictions

• Left for homework
  – Run a variety of disorder predictions on Interleukin7

• Bonus exercise
  – look for available structure data to evaluate predictions
DAY 1 WRAPUP
Ensembl – new in Jalview 2.10

- Principal source for
  - Reference genomes
  - Transcripts
  - Protein products

- Sequence variants
Genome -> 3D Structure
2.10 – Accurate Uniprot <> PDB mapping for multimers

SEC2_YEAST
Asymetic homodimer

NW map picks ‘best’ chain(s)
SIFTS explicitly maps all chains
Thanks!

- Feedback forms
  - See your email
- Any more questions, problems, calls for help?

Interested in trying new features?
Interested in helping develop them?

Join jalview-discuss

Sign up at issues.jalview.org