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Day 2 - Tuesday

- 09:00-10:30 Advanced Jalview and Jalview Hackathon
- 10:30-11:00 Coffee/Tea Break

11:00-12:30 Advanced Jalview and Jalview Hackathon continued

- 12:30-13:30 Lunch
- 13:30-15:00 Jalview Clinic and Jalview Hackathon
- 15:00-15:30 Coffee/Tea Break
- 15:30-15:50 Jalview Clinic and Jalview Hackathon continued

15:50-16:15 Wrap-up

16:15 Departure

Course materials

Everything is (or will) be online at <u>http://www.jalview.org/tutorial/training-materials/</u>2013/EBI/Jan/

- These slides
- Jalview v2.8 Tutorial (v1.4.1)
- A copy of the tutorial is also on Penelope

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



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
 - make sure you are using the latest 2.8 Build

- Verify retrieval by examining sequence annotation

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
- Question
 - What happens if only a subsequence is present in the alignment ?
 - Does database annotation get shared between alignments ?

Sequence Features



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 ?

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 31 and 32 (Sec 2.9.4)

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

Shading, thresholding, colour by label.



Working with sequence features Ex 31 and 32 (Sec 2.9.4)

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

Protein secondary structure prediction

Section 2.6 onwards in the Manual Page 64

Protein Secondary Structure Prediction Sect 2.6

- Jalview interfaces with the Jpred protein secondary structure predictor
- Prediction is based on
 - Neural net which can recognise helical, coil or beta strand using amino acid patterns
 - Amino acid profile for a sequence
 - Multiple sequence alignment
 - Profile from sequence database search
 - Position Specific Substitution Matrix

Protein Secondary Structure Prediction Sect 2.6



Exercise 26

- Tasks
 - Perform a variety of Jnet predictions
 - Note the effect of hidden regions
 - Learn about sequence associated annotation
 - Save your results for the next exercise
- Questions

Exercise 26

- Tasks
 - Perform a variety of Jnet predictions
 - Note the effect of hidden regions
 - Learn about sequence associated annotation
 - Save your results for the next exercise
- 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 ?

Alignment Annotation and sequence features.



Creating, editing and using annotation. Exercise 28 (Sec. 2.8.4)

- Tasks
 - Manually annotate some columns using the interactive editing functions
 - Learn about jalview annotation files
 - How to change the appearance of quantitative data.
 - Understand how to create sequence associated annotation
- Questions
 - What other things can be defined in jalview annotation files ?

- Session 3
 - Sequence DB refs and Sequence Features
 - Protein secondary structure prediction
 - Alignment annotation
- Session 4
 - Working with structures
 - Viewing 3D structures
 - Viewing RNA

Protein Structure and Jalview Section 2.1

- Jalview includes the Jmol molecular graphics viewer
 - Structures can be coloured by their aligned sequences
 - Position of mouse highlighted in sequence or structure

Structure shaded by sequence



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



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 ?

Colouring structures using many multiple alignments Sect 2.1.5. Exercise 16



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

Protein Feature visualization on DNA Section 2.10, exercise 33

- Task
 - Retrieve a DNA contig and visualize features from UNIPROT at their coding positions.
- Question
 - What fields in an EMBL sequence record can Jalview use ?

Semantic Processing: Database Reference Tracing

'get me the sequences from database **blah** for the selected sequences'



Jalview 2.8 and RNA 2nd-ary Structure





WRAP UP









18 new alignment conservation calculations provided as web services



T-COFFEE alignment reliability scores



Disorder Predictions from JABAWS



Disorder in Interleukin 7







<u>The Jalview</u> <u>developers</u> **Michele Clamp** *Harvard, USA.*



James Cuff Harvard, USA.

Steve Searle



Andrew Waterhouse Basel, Switzerland. <u>RNA Features</u> Lauren Lui UC Santa Cruz, USA. Jan Engelhardt

Univ. Leipzig, Germany. Yann Ponty (**VARNA**)



<u>T-COFFEE Scores</u> **Paolo di Tomasso** *Notredame Group, CRG, Spain.* Geoff Barton (**Money**) David Martin (**Teaching**) Peter Troshin (**JABAWS**) Barry Strachan (**Iogo**) Tom Walsh (**Apache**) Ryan Maclaughlan (**CSS**) Andrew Millar (**Drupal**)

All the Jalview users, and

