



H3ABioNet

Pan African Bioinformatics Network for H3Africa

Introduction to Bioinformatics online course: IBT

Multiple Sequence Alignment

Lec6:Selecting and editing sequences

By

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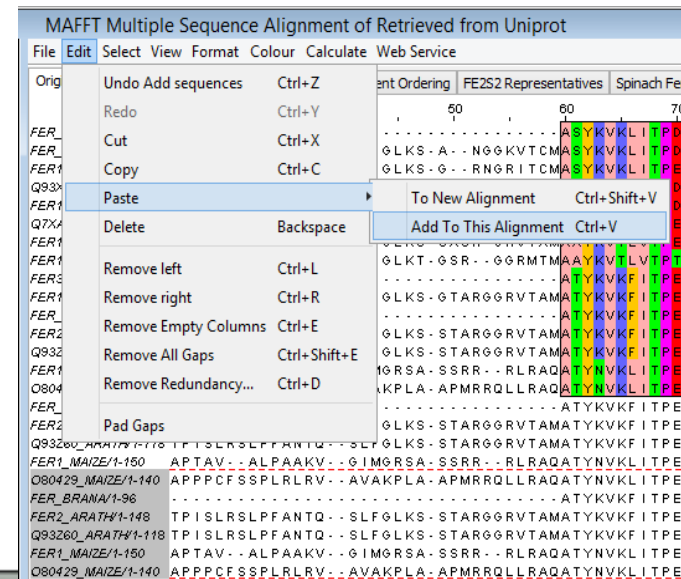
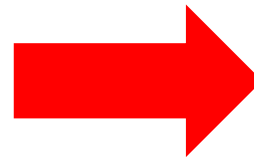
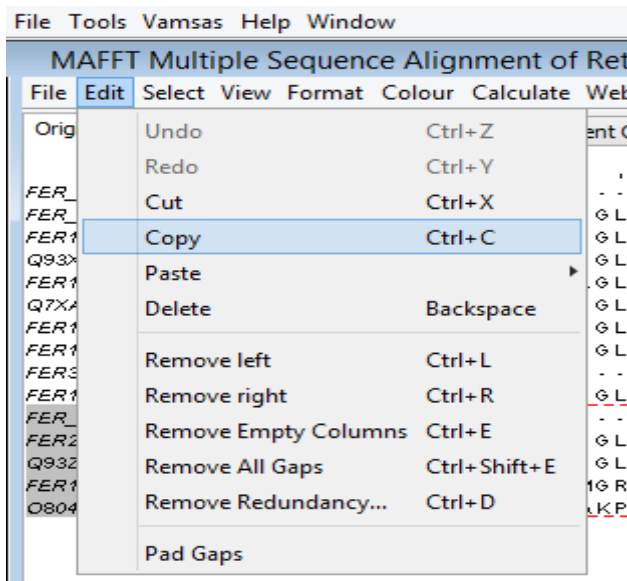
Selecting and editing sequences

Selecting parts of an alignment

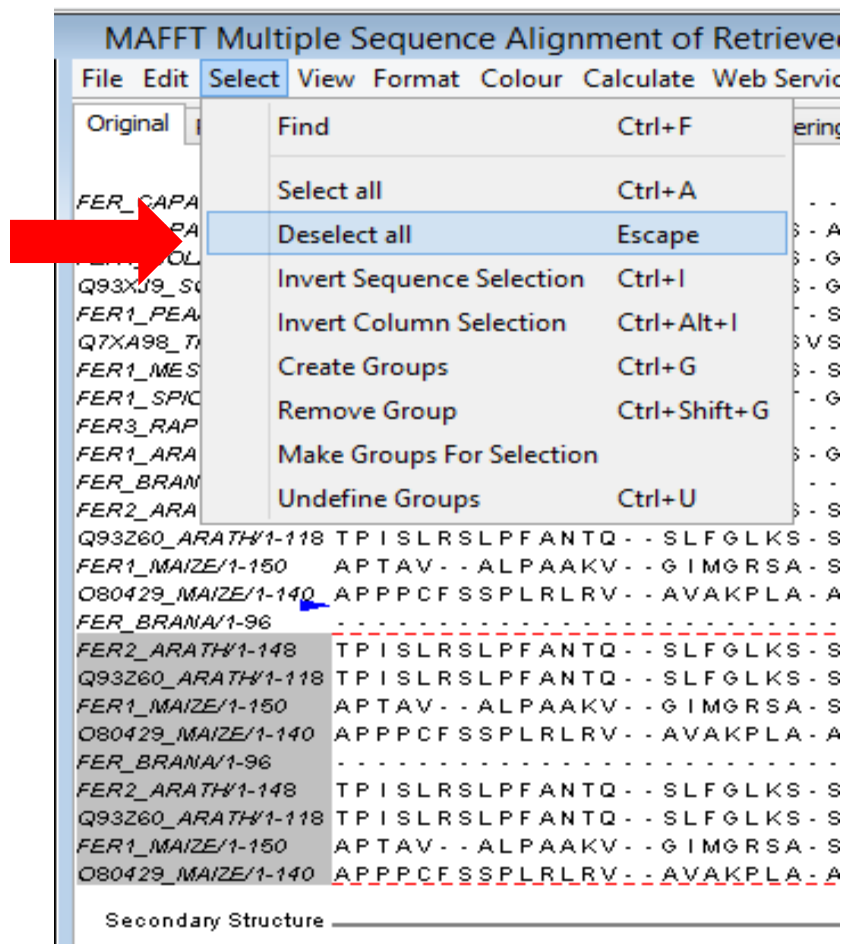
Selections can be of **arbitrary regions** in an alignment, one or more **complete columns**, or one or more **complete sequences**.

A **selected region** can be copied and pasted as a new alignment using the:

Edit ⇒ Copy and Edit ⇒ Paste ⇒ To New Alignment
in the alignment window menu options..

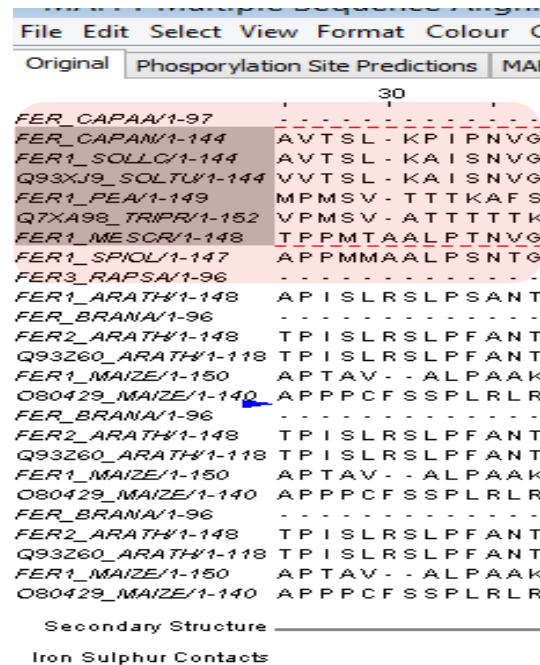


To clear (**Deselect**) the selection press the [**ESC**] (**Escape**) key



Selecting arbitrary regions

To select part of an alignment, place the mouse at the **top left corner** of the region you wish to select. **Press and hold** the mouse button and **drag** the mouse to the **bottom right corner** of the chosen region then release the mouse button. A dashed red box appears around the selected region. **Selecting a region in an alignment**



Selecting columns

- To select the **same residues** in **all sequences**, **click and drag along** the alignment **ruler**. This selects the entire height of the alignment.
- **Ranges of positions** can also be selected by **clicking on the first** position then **holding down** the **[SHIFT]** key whilst **clicking the other end** of the selection.
- **Discontinuous regions** can be selected by **holding down [CTRL]** and **clicking on positions to add** to the column selection. Note that each **[CTRL]** Selected columns are indicated by red highlighting in the ruler bar

MAFFT Multiple Sequence Alignment of Retrieval

File Edit Select View Format Colour Calculate Web Services

Original	Phosphorylation Site Predictions	MAFFT Alignment Order
	20	30
FER_CAPAA/1-97	4
FER_CAPAN/1-144	TSFMPRKPAVTSL-KPIPNVGE	
FER1_SOLLG/1-144	TSFLPRKPAVTSL-KAISNVGE	
Q93XJ9_SOLTUV/1-144	TSFLPRKPVVTSL-KAISNVGE	
FER1_PEA/1-149	TSFLRTQPMPSV-TTTKAFSN	
Q7XA98_TRIPR/1-152	TSFMRRQVPVMSV-ATTTTAKAF	
FER1_MESCR/1-148	TAFAPK--TPPMTAALPTNVGR	
FER1_SPIOL/1-147	TTFVPKPKQAPPMMMAALPSNTGR	
FER3_RAPSA/1-96	
FER1_ARATH/1-148	TSFIRRSPAPISLRSLSANTQ	
FER_BRANA/1-96	

File Tools Vamsas Help Window

MAFFT Multiple Sequence Alignment

File Edit Select View Format Colour Cal

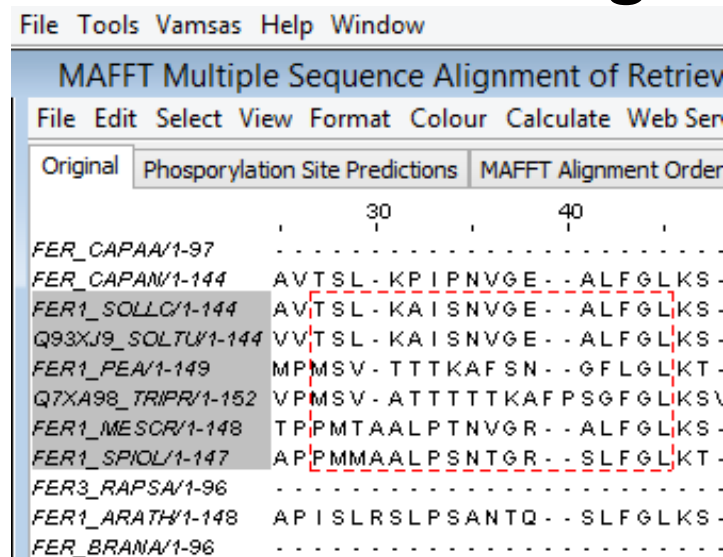
Original	Phosphorylation Site Predictions	MAFFT
	20	30
FER_CAPAA/1-97	
FER_CAPAN/1-144	TSFMPRKPAVTSL-	
FER1_SOLLG/1-144	TSFLPRKPAVTSL-	
Q93XJ9_SOLTUV/1-144	TSFLPRKPVVTSL-	
FER1_PEA/1-149	TSFLRTQPMPSV-	
Q7XA98_TRIPR/1-152	TSFMRRQVPVMSV-	
FER1_MESCR/1-148	TAFAPK--TPPMTA	
FER1_SPIOL/1-147	TTFVPKPKQAPPMM	
FER3_RAPSA/1-96	
FER1_ARATH/1-148	TSFIRRSPAPISLR	
FER2_ARATH/1-148	TSFLRRRQQTPISLR	
Q93260_ARATH/1-118	TSFLRRRQQTPISLR	
FER1_MAIZE/1-150	SSSLRAAPAPTAV-	
O80429_MAIZE/1-140	MSILR--APPPCF	
FER_BRANA/1-96	
FER2_ARATH/1-148	TSFLRRRQQTPISLR	
Q93260_ARATH/1-118	TSFLRRRQQTPISLR	
FER1_MAIZE/1-150	SSSLRAAPAPTAV-	
O80429_MAIZE/1-140	MSILR--APPPCF	

Secondary Structure

Iron Sulphur Contacts

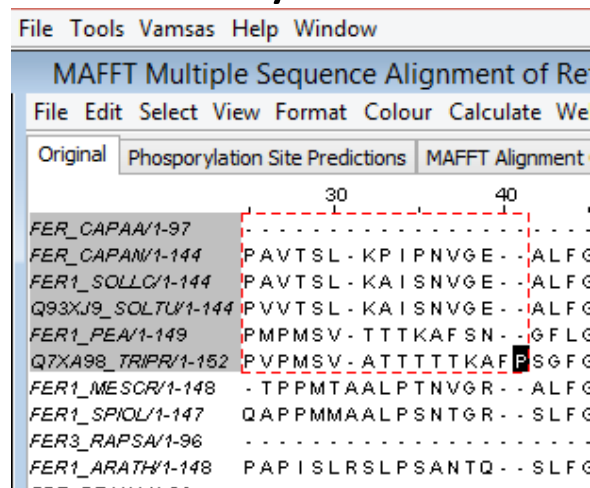
Selecting sequences

To select **multiple complete sequences**, click and **drag** the mouse **down** the sequence **ID panel**. The same technique as used for columns above can be used with **[SHIFT]-Click** for **continuous** and **[CTRL]-Click** to select **discontinuous** ranges of sequences.



Making selections in Cursor mode

To define a selection in cursor mode (which is enabled by pressing **[F2]** when the alignment window is selected), navigate to the top left corner of the proposed selection (using the mouse, the arrow keys, or the keystroke commands described). Pressing the **[Q]** key **marks** this as the **corner**. A red outline appears around the cursor. Navigate to the **bottom** right corner of the proposed selection and press the **[M]** key. This marks the bottom right corner of the selection. The selection can then be treated in the same way as if it had been created in normal mode.



Inverting the current selection

The current sequence or column selection can be inverted, using **Select ⇒ Invert Sequence/Column Selection** in the alignment window.

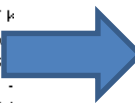
Inverting the selection is useful when selecting large regions in an alignment, simply select the region that is to be kept unselected, and then invert the selection.

MAFFT Multiple Sequence Alignment of Retrieved from Uni

File Edit Select View Annotations Format Colour Calculate

Original MAFFT Alignment Ordering Spinach Ferredoxin Structure FE

	30	40	50
FER_CAPAA/1-97
FER_CAPAN/1-144	AVTSL·KPIPNVGE··ALFGLKS·A··
FER1_SOLLC/1-144	AVTSL·KAISNVGE··ALFGLKS·G··
Q93XJ9_SOLTU/1-144	VVTSL·KAISNVGE··ALFGLKS·G··
FER1_PEA/1-149	MPMSV·TTTKAFSN··GFLGLKT·SLK
Q7XA98_TRIPR/1-152	VPMSV·ATTTTAKAFPSGFLGLKS·VSTK
FER1_MESCR/1-148	TPPMTAALPTNVGR··ALFGLKS·SA
FER1_SPIOL/1-147	APPMMAALPSNTGR··SLFGLKT·GS
FER3_RAPSA/1-96
FER1_ARATH/1-148	APISLRSPLPSANTQ··SLFGLKS·GTA
FER_BRANA/1-96
FER2_ARATH/1-148	TPISLRSPLPFANTQ··SLFGLKS·STA
Q93Z60_ARATH/1-118	TPISLRSPLPFANTQ··SLFGLKS·STA
FER1_MAIZE/1-150	APTAV··ALPAAKV··GIMGRSA·SSF
O80429_MAIZE/1-140	APPPCFSSPLRLRV··AVAKPLA·APN



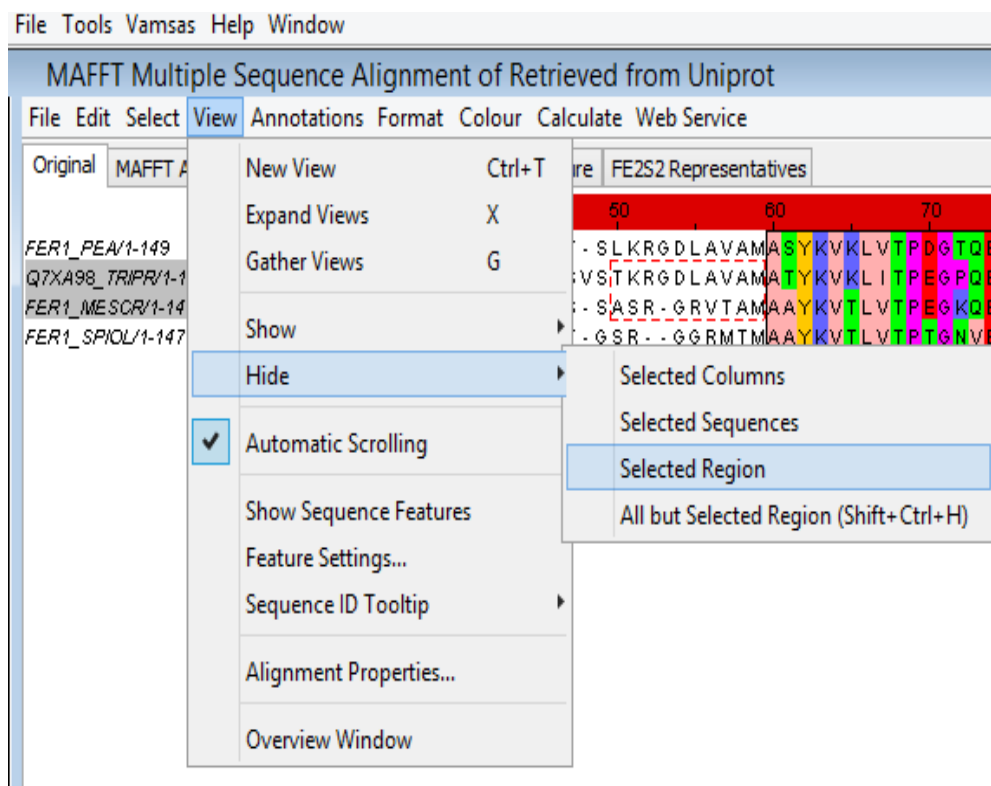
MAFFT Multiple Sequence Alignment of Retrieved from Uni

File Edit Select View Annotations Format Colour Calculate Web Servi

Original MAFFT Alignment Ordering Spinach Ferredoxin Structure FE2S2 Repres

	30	40	50
FER_CAPAA/1-97
FER_CAPAN/1-144	AVTSL·KPIPNVGE··ALFGLKS·A··
FER1_SOLLC/1-144	AVTSL·KAISNVGE··ALFGLKS·G··
Q93XJ9_SOLTU/1-144	VVTSL·KAISNVGE··ALFGLKS·G··
FER1_PEA/1-149	MPMSV·TTTKAFSN··GFLGLKT·SLK
Q7XA98_TRIPR/1-152	VPMSV·ATTTTAKAFPSGFLGLKS·VSTK
FER1_MESCR/1-148	TPPMTAALPTNVGR··ALFGLKS·SA
FER1_SPIOL/1-147	APPMMAALPSNTGR··SLFGLKT·GS
FER3_RAPSA/1-96
FER1_ARATH/1-148	APISLRSPLPSANTQ··SLFGLKS·GTA
FER_BRANA/1-96
FER2_ARATH/1-148	TPISLRSPLPFANTQ··SLFGLKS·STA
Q93Z60_ARATH/1-118	TPISLRSPLPFANTQ··SLFGLKS·STA
FER1_MAIZE/1-150	APTAV··ALPAAKV··GIMGRSA·SSF
O80429_MAIZE/1-140	APPPCFSSPLRLRV··AVAKPLA·APN

This may also be useful when hiding large regions in an alignment. Instead of selecting the columns and rows that are to be hidden, simply select the region that is to be kept visible, invert the selection, then select **View ⇒ Hide ⇒ Selected Region**.



Creating groups

Selections are lost as soon as a **different region is selected**. Groups can be created which are **labeled regions** of the alignment.

To create a group,

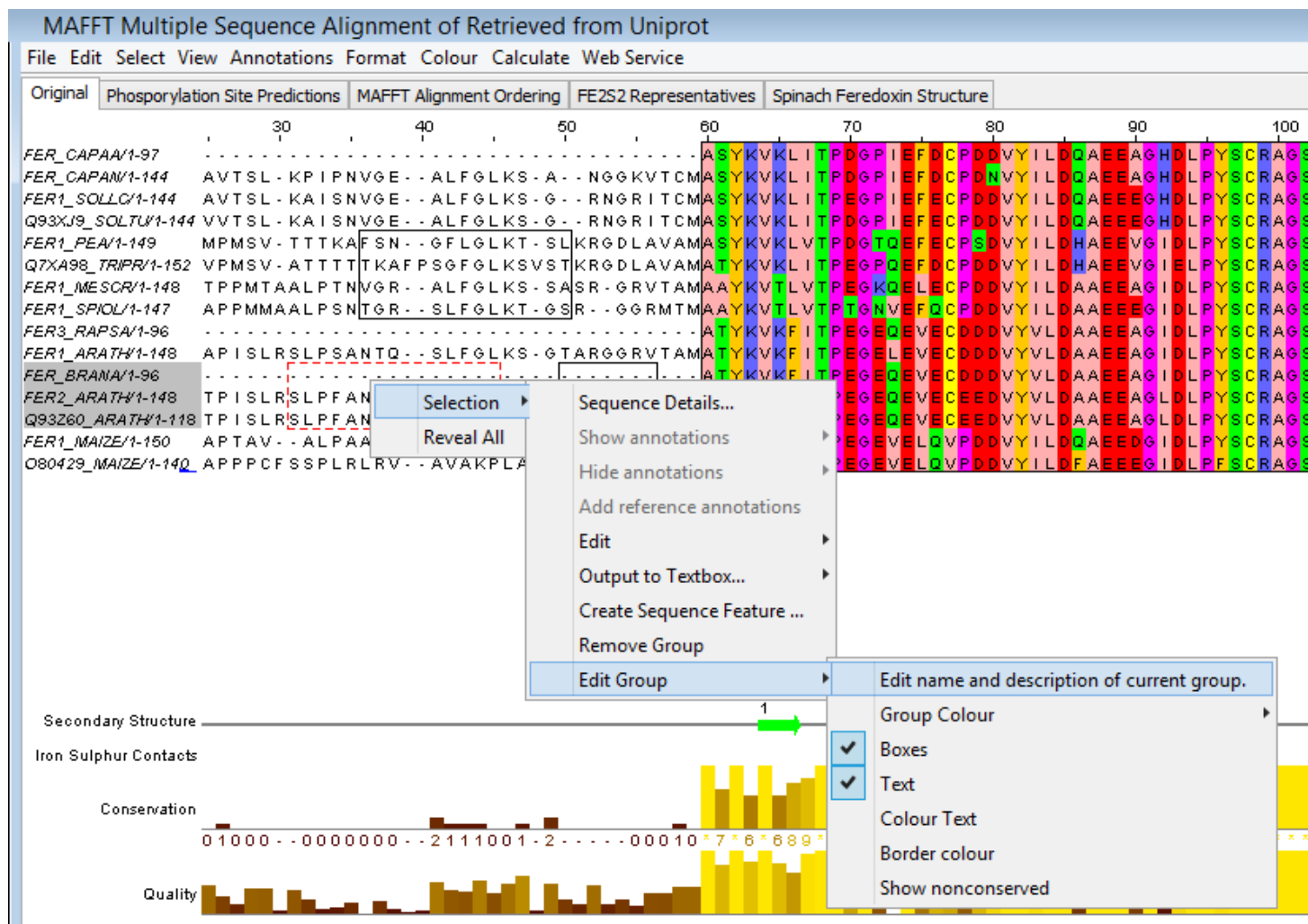
- **first select the region** which is to comprise the group.
- **Then click the right mouse** button on the selection to bring up a context menu.

Select ***Selection ⇒ Group ⇒ Edit***

- ***name and description of current group***15
- then enter a name for the group in the dialogue box which appears.

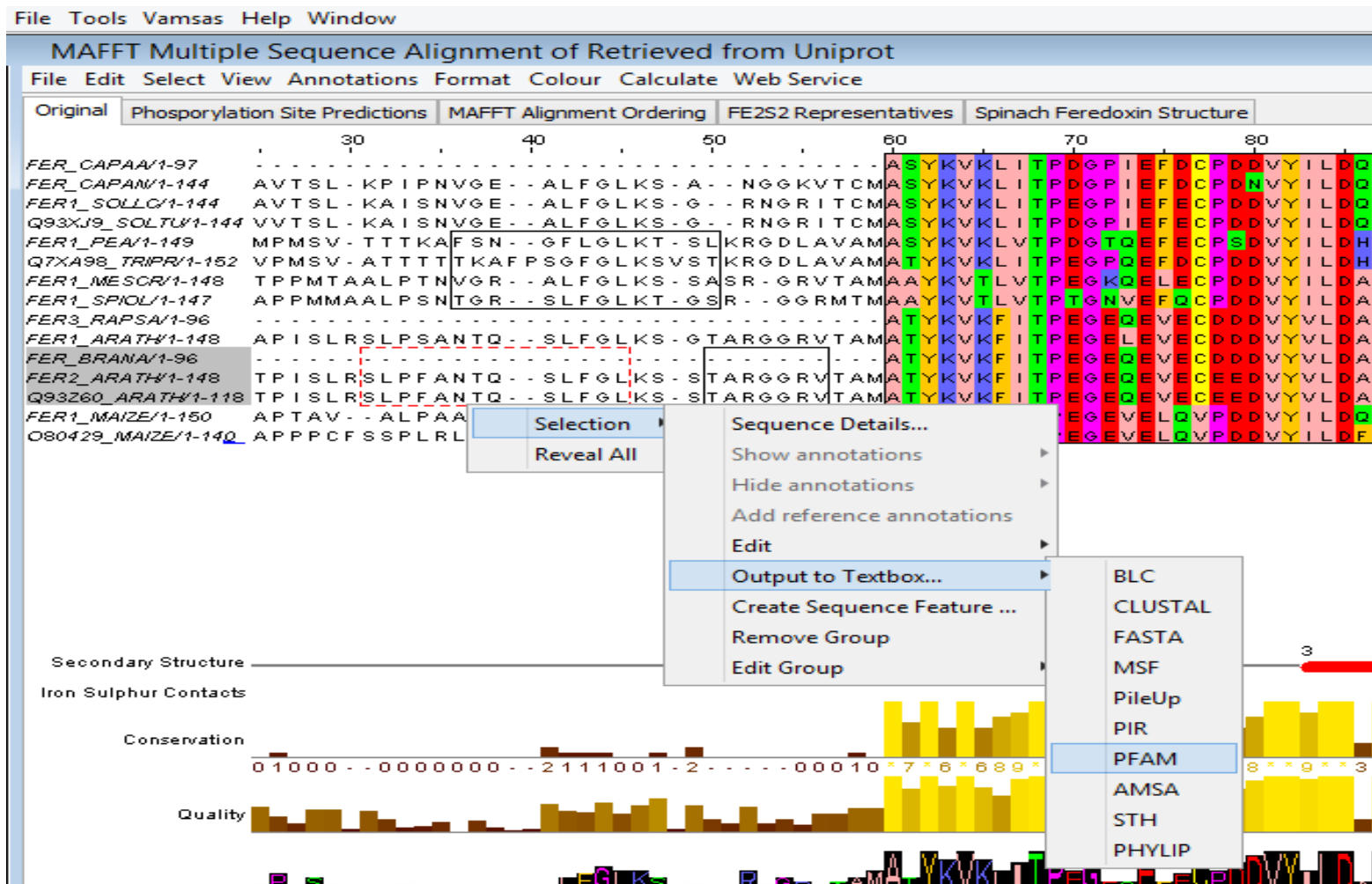
By default the new group will have a box drawn around it. The appearance of the group can be changed .

This group will stay defined even when the selection is removed.



Exporting the current selection

- The **current selection** can be copied to the **clipboard** (in PFAM format).
- It can also be **output to a textbox** using the output functions in the pop-up menu obtained by right clicking the current selection.
- The **textbox enables** quick manual editing of the alignment prior to importing it into a new window (using the [New Window] button) or saving to a file with the *File ⇒ Save As* pulldown menu option from the text box.



AACon Protein Alignment Conservation Services

Jalview 2.9.0b2

File Tools Vamps Help Window

http://www.jalview.org/tutorial/unaligned.fa

File Edit Select View Annotations Format Colour Calculate Web Service

Alignment
Secondary Structure Prediction
Protein Disorder
Analysis
Conservation
Fetch DB References

AACon Calculations
Change AACon Settings...

Modify settings for AACon calculations...

Conservation
Quality
Consensus
SHENHON

Sequence 1 ID: FER_CAPAA Residue: SER (43)

Web Services >> Conservation >> Change AACon Settings

Jalview 2.9.0b2

File Tools Vampsas Help Window

http://www.jalview.org/tutorial/unaligned.fa

File Edit Select View Annotations Format Colour Calculate Web Service

10 20 30 40 50 60 70 80 90

FER_CAPAA/1-97 ASYKVKLITPDPIEFDCDDVYILDQAEAGHDLFYSCRAQSCSSCAQKIAQGAVDQTDONFLDDQLEEGWVLTCAVYQSDVTIETHKEAE

FER_CAPAA/1-144 MASVSATMISTFMPKPAVTSKLPINVGAEALFGLKSANGKVTCTMASYKVKLITPDPIEFDCDDVYILDQAEAGHDLFYSCRAQSCSSCA

FER1_SQLO/1-144 MASISQTMISTFMPKPAVTSKLPINVGAEALFGLKSANGKVTCTMASYKVKLITPDPIEFDCDDVYILDQAEAGHDLFYSCRAQSCSSCA

Q93XJ9_SQLO/1-144 MASISQTMISTFMPKPAVTSKLPINVGAEALFGLKSANGKVTCTMASYKVKLITPDPIEFDCDDVYILDQAEAGHDLFYSCRAQSCSSCA

FER1_PEA/1-149 MATTPALYGTAVTSFMRQPPVMSVATTTTAKFNGFLGLKTSKRGDLAVAMASYKVKLVTPDGTQEFECPSDVYILDHAEVGLDLYSCRAQ

Q7XA96_TRIP/1-152 MATTPALYGTAVTSFMRQPPVMSVATTTTAKFNGFLGLKTSKRGDLAVAMASYKVKLVTPDGTQEFECPSDVYILDHAEVGLDLYSCRAQ

FER1_MESCR/1-148 MAATTAALSQATMSTAFAPKTPMTAALPTNVGRALFGLKSASGRVTAMAAKVTLVTPDGTQEFECPSDVYILDHAEVGLDLYSCRAQ

FER1_SQLO/1-147 MAATTTTMMQMATTFVPPQAPPMMAALPNTORSLFGLKTSKRGDLAVAMASYKVKLVTPDGTQEFECPSDVYILDHAEVGLDLYSCRAQ

FER1_RAPSA/1-96 ATYKVKFITPEGEVECEDDVYVLDAAEEAGIDLPYSCRAQSCSSCAQKVVSGVDQSDSFLDDQIAEGFVLTCAAYPTSDVTIETHKEAE

FER1_ARATH/1-98 MASTALSSAIVSTFIRRSAPISLRSPLFANTQSLFGLKTSKRGDLAVAMASYKVKLVTPDGTQEFECPSDVYILDHAEVGLDLYSCRAQ

ATYKVKFITPEGEVECEDDVYVLDAAEEAGIDLPYSCRAQSCSSCAQKVVSGVDQSDSFLDDQIAEGFVLTCAAYPTSDVTIETHKEAE

FER2_ARATH/1-148 MASTALSSAIVSTFIRRSAPISLRSPLFANTQSLFGLKTSKRGDLAVAMASYKVKLVTPDGTQEFECPSDVYILDHAEVGLDLYSCRAQ

Q93Z60_ARATH/1-118 MASTALSSAIVSTFIRRSAPISLRSPLFANTQSLFGLKTSKRGDLAVAMASYKVKLVTPDGTQEFECPSDVYILDHAEVGLDLYSCRAQ

FER1_MAIZE/1-150 MATVLGSPRAPAFFSSSSSLRAAPATAVALPAKVGIMGRSASSRRRLRAQATYNVKLITPEGEVECEDDVYVLDAAEEAGIDLPYSCRAQ

Q00429_MAIZE/1-140 MAATLQMSILRAPPCFSSPLRLRVAVAKPLAAMPRLRLRAQATYNVKLITPEGEVECEDDVYVLDAAEEAGIDLPYSCRAQSCSSCAQK

Conservation

Quality

Consensus

SHENKIN

Sequence 1 ID: FER_CAPAA Residue: SER (43)

Edit parameters for Conservation with AACONWS

Current parameter set name: Defaults

Details

Options

☐ ARMON
 ☐ GERSTEIN
 ☐ JORES
 ☐ KABAT
 ☐ KARLIN
 ☐ LANDGRAF
 ☐ MIRNY
 ☐ NOT_LANCET
 ☐ SANDER
 ☐ SCHNEIDER
 ☒ SHENKIN
 ☐ SMERFS
 ☐ TAYLOR_GAPS
 ☐ TAYLOR_NO_GAPS
 ☐ THOMPSON
 ☐ VALDAR
 ☐ WILLIAMSON
 ☐ ZVELIBIL
 ☒ Normalize

Parameters

SMERFS Column Scoring Method

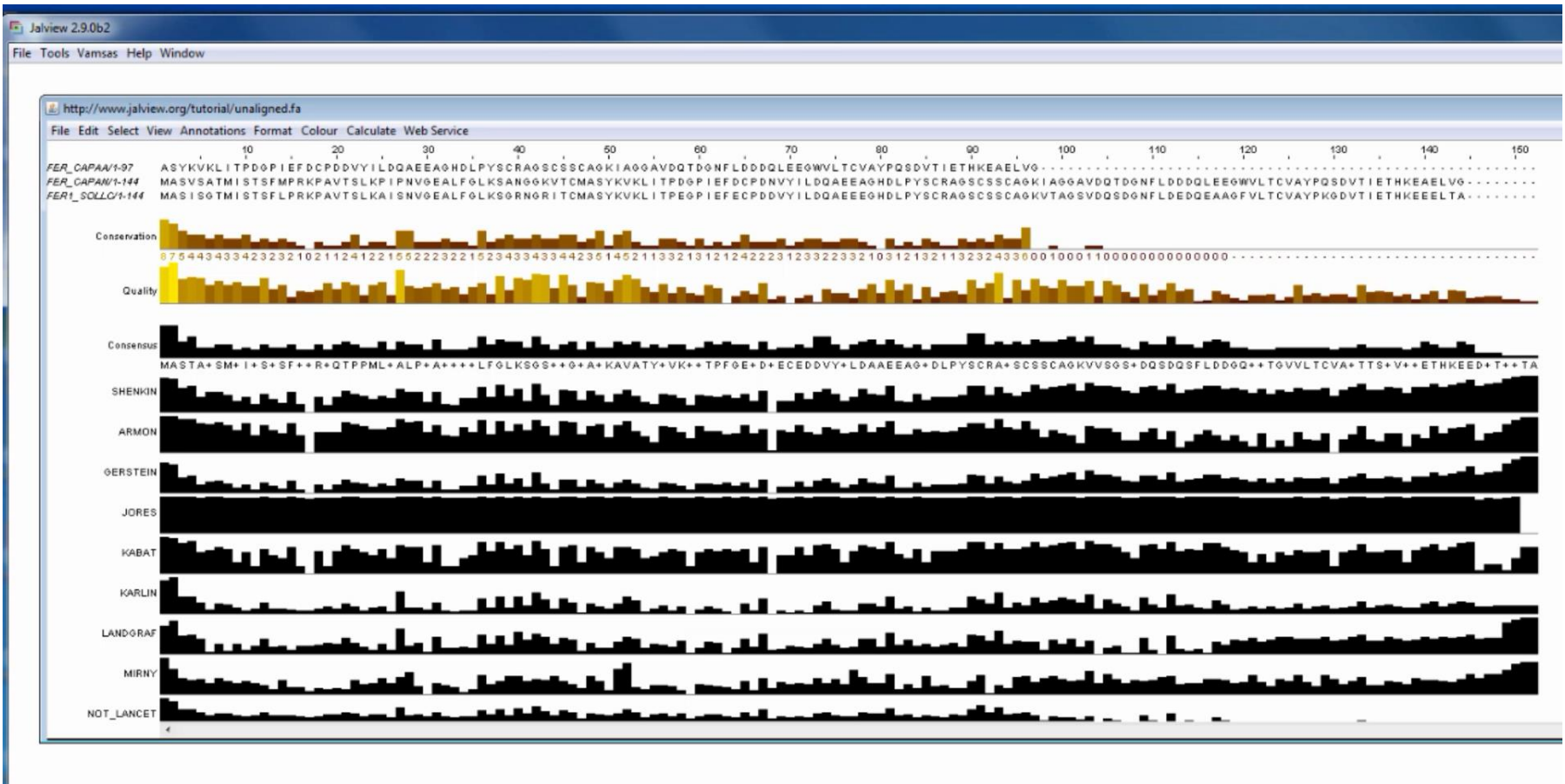
MID_SCORE

SMERFS Gap Threshold

0.1

SMERFS Window Width

7



Practical

“To try on your own time”

Exercise : Making selections and groups

- 1- Close all windows in Jalview and load the ferredoxin alignment (**PFAM ID PF03460**).
- 2- Choose a residue and place the mouse cursor on it. Click and drag the mouse cursor to create a selection. As you drag, a red box will 'rubber band' out to show the extent of the selection. Release the mouse button and a red box should border the selected region.
- 3 - Now press [**ESC**] to clear the selection.
 - Select one sequence by clicking on the ID panel. Note that the sequence ID takes on a highlighted background and a red box appears around the selected sequence.
 - Now hold down [**SHIFT**] and click another sequence ID a few positions above or below. Note how the selection expands to include all the sequences between the two positions on which you clicked.
 - Now hold down [**CTRL**] and click on several sequences ID's both selected and unselected. Note how unselected IDs are individually added to the selection and previously selected IDs are individually deselected.
- 4- Repeat the step above but selecting columns by clicking on the ruler bar instead of selecting rows by clicking on the sequence ID.
- 5- Press [**F2**] to enter Cursor mode. Navigate to column 59, row 1 by pressing 5 9 , 1 [**RETURN**].

- Press **Q** to mark this position. Now navigate to column 65, row 8 by pressing **6 5 , 8 [RETURN]**. Press **M** to complete the selection.
- Open the popup menu by right-clicking the selected region with the mouse. Open the **Selection ⇒ Group ⇒ Group Colour** menu and select 'Percentage Identity'.
- This will turn the selected region into a group and color it accordingly.
- Hold down [**CTRL**] and use the mouse to select and deselect sequences by clicking on their Sequence ID label. Note how the group expands to include newly selected sequences, and the 'Percentage Identity' coloring changes.
- Use the mouse to click and drag the right-hand edge of the selected group. Note again how the group resizes.

Right click on the text area to open the selection popup-menu. Follow the menus and pick an output format from the **Selection ⇒ Output to Textbox . . .** submenu. Try manually editing the alignment and then press the [**New Window**] button to import the file into a new alignment window.

BTU BIOINFORMATICS TRAINING UNIT



Bioinformatics Workshops Series

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- 2nd Module: Manipulation of Biological Sequences
- 3rd Module: Working with single DNA sequence
- 4th Module: How to Build a Multiple Sequence Alignment?
- 5th Module: Inferring Phylogenetic analysis using Jellview
- 6th Module: Advanced Molecular Concepts
- 7th Module: Inferring Protein Sequence (Structure & Function)
- 8th Module: RNAanalysis and Function
- 9th Module: Editing and Publishing Alignments in your Manuscript
- 10th Module: Building and Publishing Phylogenetic Trees
- 11th Module: Working with Protein 3-D Structures
- 12th Module: Advanced Bioinformatics Using R

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