

KNIME workflow with the reporting functionality manual

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1. KNIME reporting

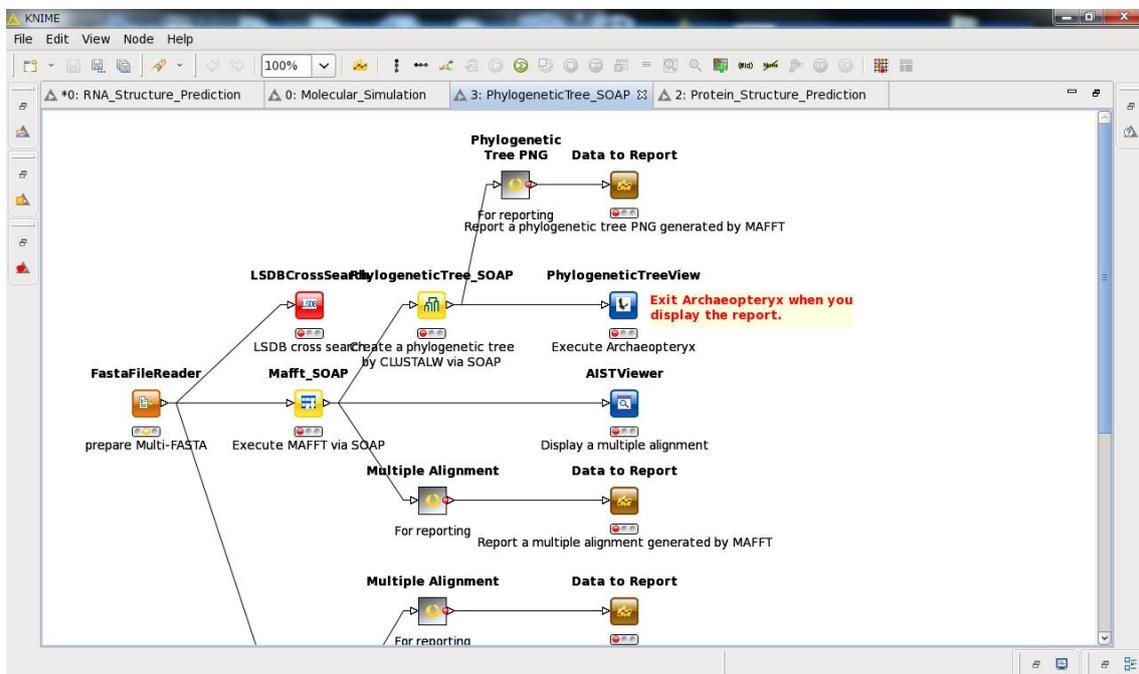
The KNIME can provide report templates for each of workflows using Eclipse BIRT (<http://www.eclipse.org/birt/phoenix/>). By using this reporting functionality, various workflow results can be reported visually and comprehensively in PDF, Word format and so on.

In AIST, the user can use PhylogeneticTree_SOAP KNIME workflow which has a report template.

1.1. PhylogeneticTree_SOAP workflow with a report template

This KNIME workflow is added the report template to existing PhylogeneticTree_SOAP KNIME workflow. New KNIME nodes are as follows:

- Data to Report: reporting node
- Phylogenetic Tree PNG: meta nodes for reporting a phylogenetic tree.
- Multiple Alignment: meta nodes for reporting a multiple alignment



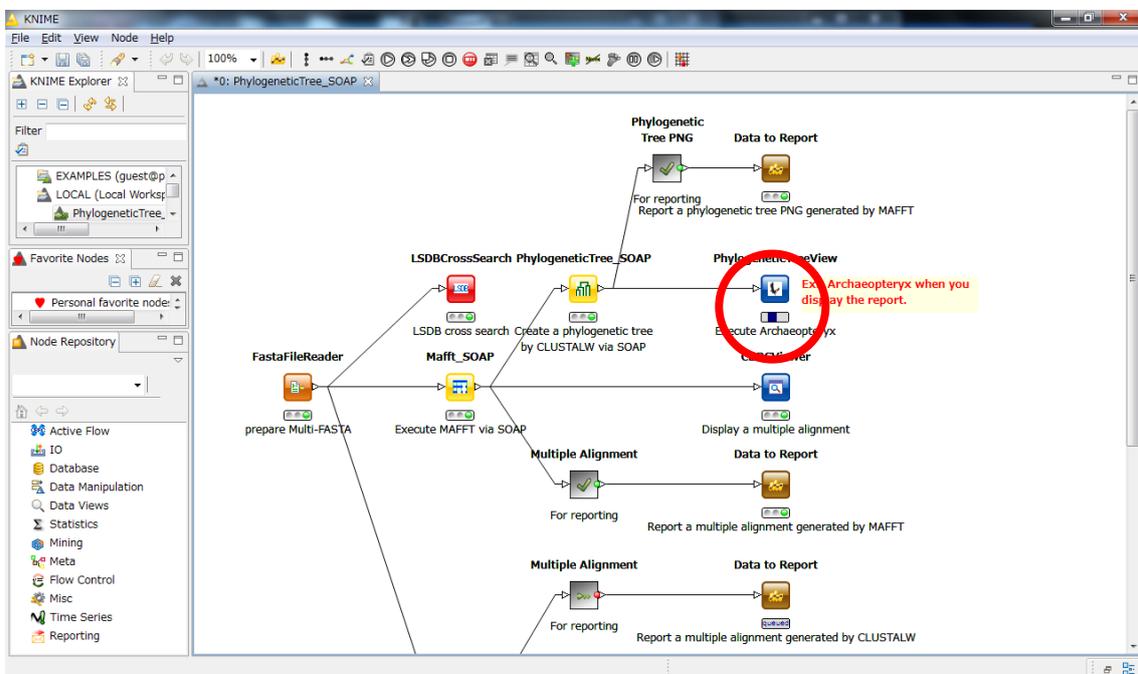
1-1 PhylogeneticTree_SOAP KNIME workflow with the report template

1.1.1. How to use the KNIME reporting

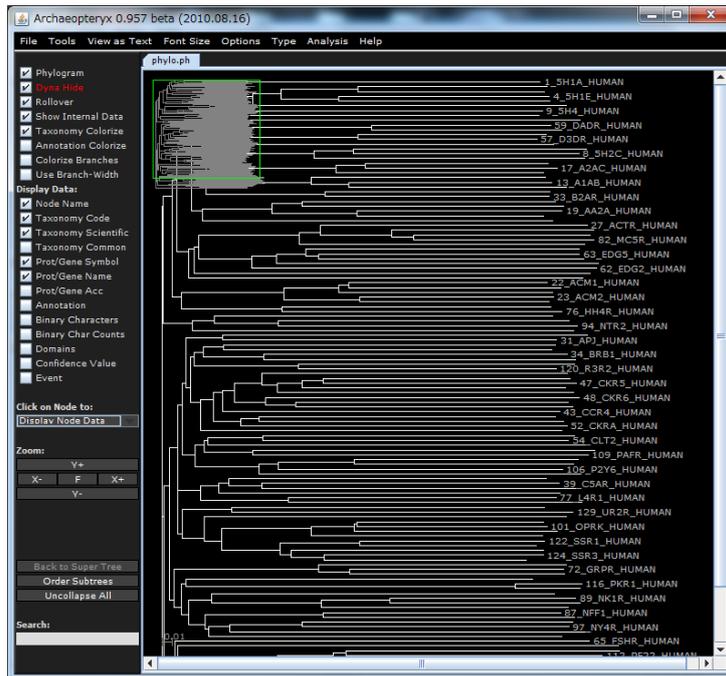
The user can use the KNIME reporting functionality in accordance with following procedures.

- 1) Except for reporting functionality, the user can execute this KNIME workflow (1-2) like existing PhylogeneticTree_SOAP. If you want to know how to use PhylogeneticTree_SOAP, please visit the PhylogeneticTree_SOAP web page (http://togo.medals.jp/active_local_phylo.eng.html).

*When the workflow execution is nearly finished, only PhylogeneticTreeView node is running and invokes an Archaeopteryx program (1-3). In PhylogeneticTree_SOAP workflow, there are two lines which generate a multiple alignment and a phylogenetic tree by Mafft_SOAP or ClustalW_SOAP, so there are two PhylogeneticTreeView nodes to display each phylogenetic tree in the workflow (the red open circle in 1-2). **If the user wants to use KNIME reporting functionality, results of the workflow should be saved. However, the results cannot be saved when any KNIME node is running. Thus, please exit Archaeopteryx program if the user want to use the reporting.**

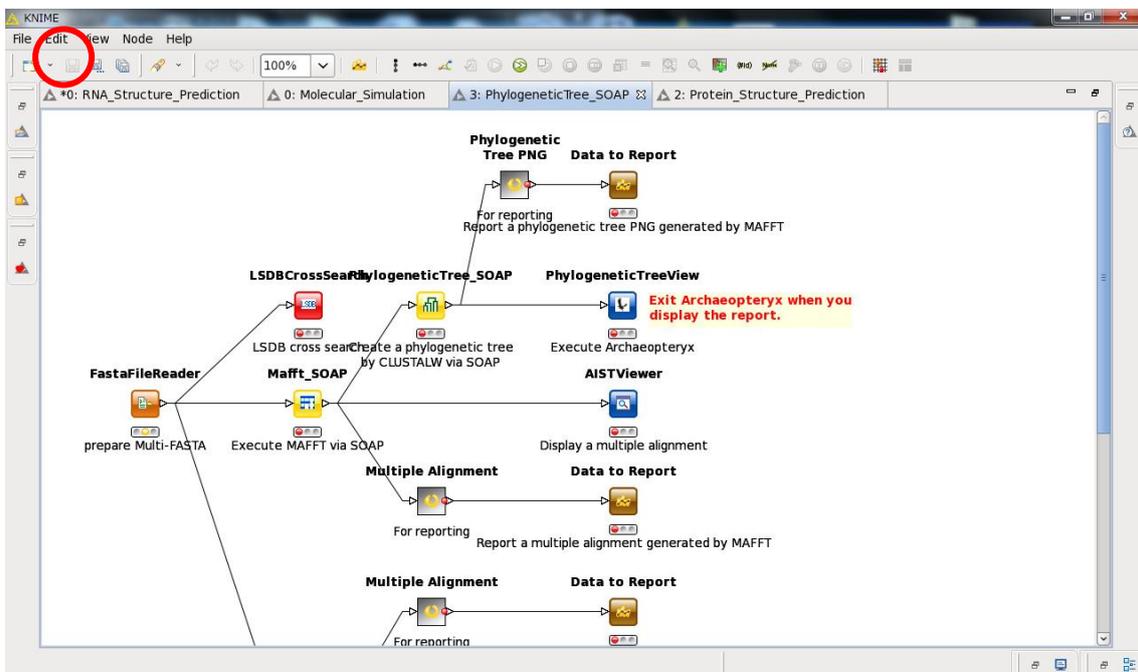


1-2 KNIME workflow (running)



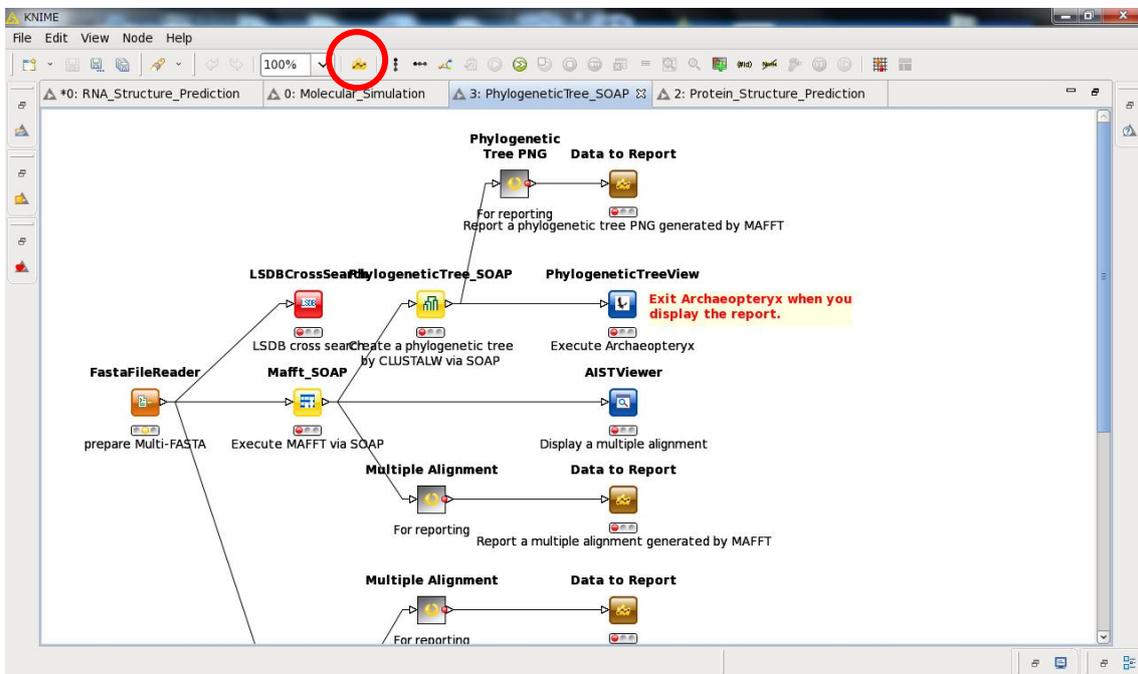
1-3 A view of phylogenetic tree by Archaeopteryx

- 2) When the user exits two Archaeopteryx programs, the KNIME workflow is completely finished (1-4). Then, the user can save results of the workflow (click on the red open circle in 1-4).



1-4 KNIME workflow (finished)

3) KNIME reporting is started (click on the red open circle in 1-5).



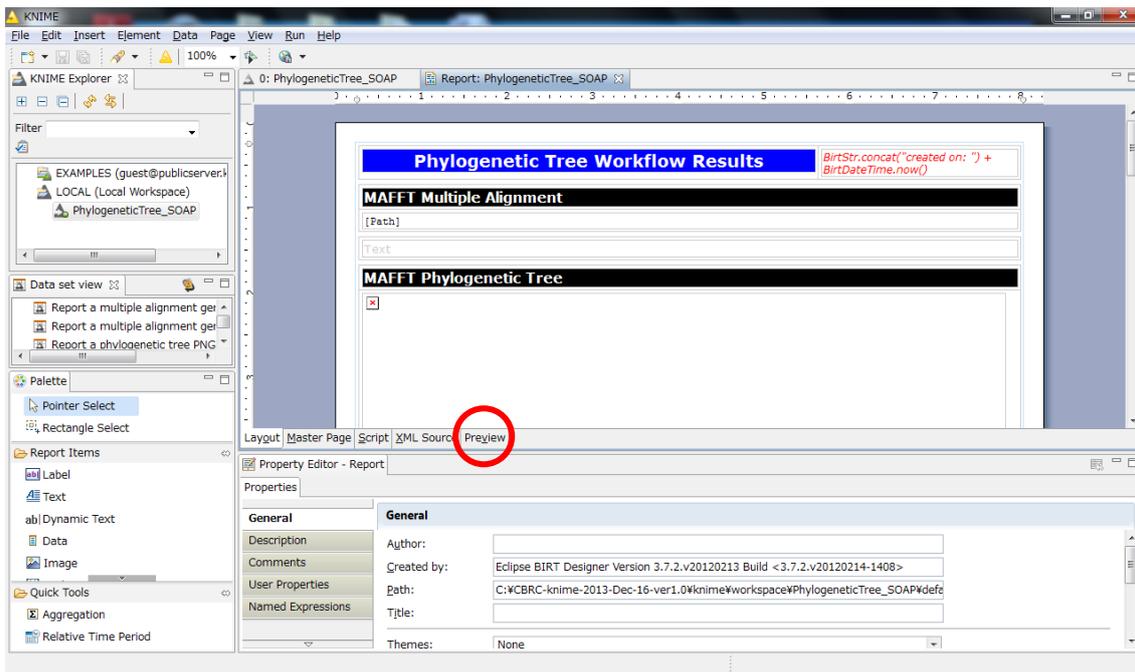
1-5 Starting KNIME reporting

4) When the layout viewing (a reporting template) of KNIME reporting is displayed, the user can click the “Preview” tab. (click on the red open circle in 1-6).

This layout viewing is a reporting template and below contents are setup in this template.

- Phylogenetic Tree Workflow Results (title)
- The date of generating the report (right hand of the title)
- Mafft Multiple Alignment (a multiple alignment result by Mafft)
- Mafft Phylogenetic Tree (a phylogenetic tree using the multiple alignment by Mafft)
- ClustalW Multiple Alignment (a multiple alignment result by ClustalW)
- ClustalW Phylogenetic Tree (a phylogenetic tree using the multiple alignment by ClustalW)

A report contained the results of the workflow is output based on the template.

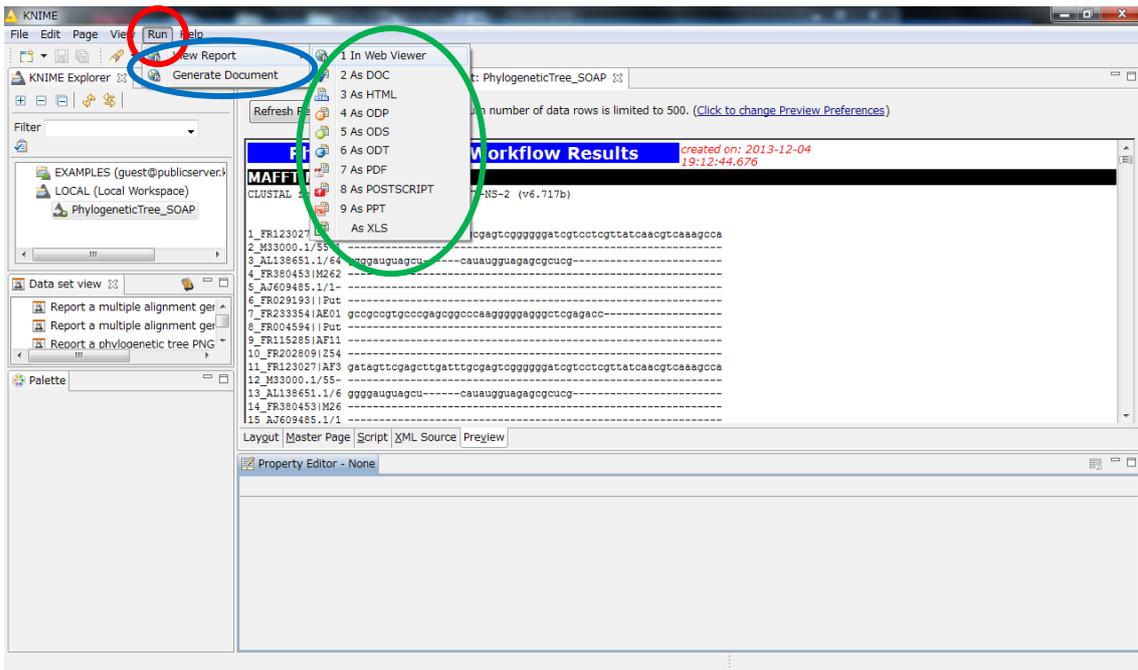


1-6 Layout viewing (the reporting template) of the KNIME reporting

5) The preview of KNIME reporting is displayed (1-7). The user can check whether the results of the KNIME workflow is correctly displayed based on the reporting template (1-6) or not. After checking, if the user select the “Run” tag from the menu bar at the top of the display (the red open circle in 1-7), ”View Report” and ”General Document” are displayed in a menu (the blue open circle in 1-7). In this case ”View Report” is selected. Then, a menu which contains various report types is opened (the green open circle in 1-7). If the user selects ”In Web Viewer”, BIRT Report Viewer is started and is displayed the report which contains the results of the workflow (1-8).

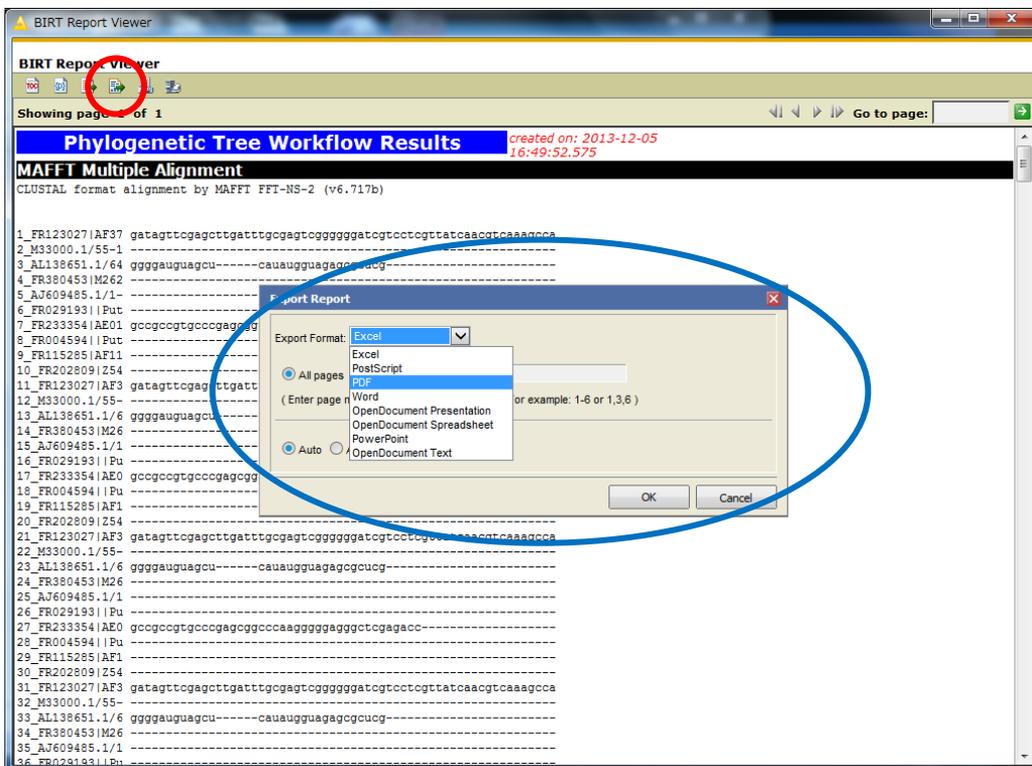
The reporting types are as follows:

- In Web Viewer (a BIRT Report Viewer)
- As DOC (a Word file format)
- As HTML (a BIRT Report Viewer)
- As ODP (an Open Document format)
- As ODS (an Open Document format)
- As ODT (an Open Document format)
- As PDF (a PDF format)
- As POSTSCRIPT (a PostScript format)
- As PPT (a Power Point format)
- As XLS (an Excel format)



1-7 Preview of the KNIME reporting

- 6) The report which contains the results of the workflow is displayed on the BIRT Report Viewer (1-8). By clicking “Export Report” icon of an icon bar at the top of the display (the red open circle in 1-8), a pop-up menu of “Export Report” is displayed (the blue open circle in 1-8) and the user can select file format to save.



1-8 BIRT Report Viewer

7) The user can open the report saved as a file and check the results of the workflow.

The screenshot shows a PDF document titled "default_report.pdf - Adobe Reader". The main content is a report titled "Phylogenetic Tree Workflow Results" with a creation timestamp of "2013-12-04 19:04:15.182".

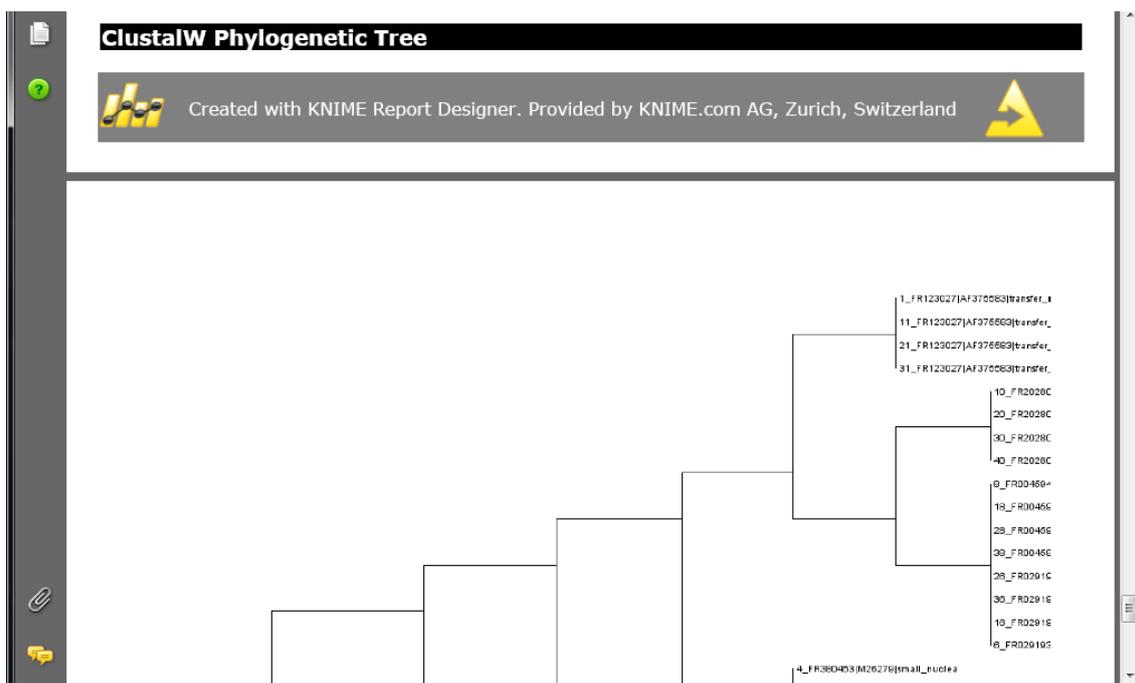
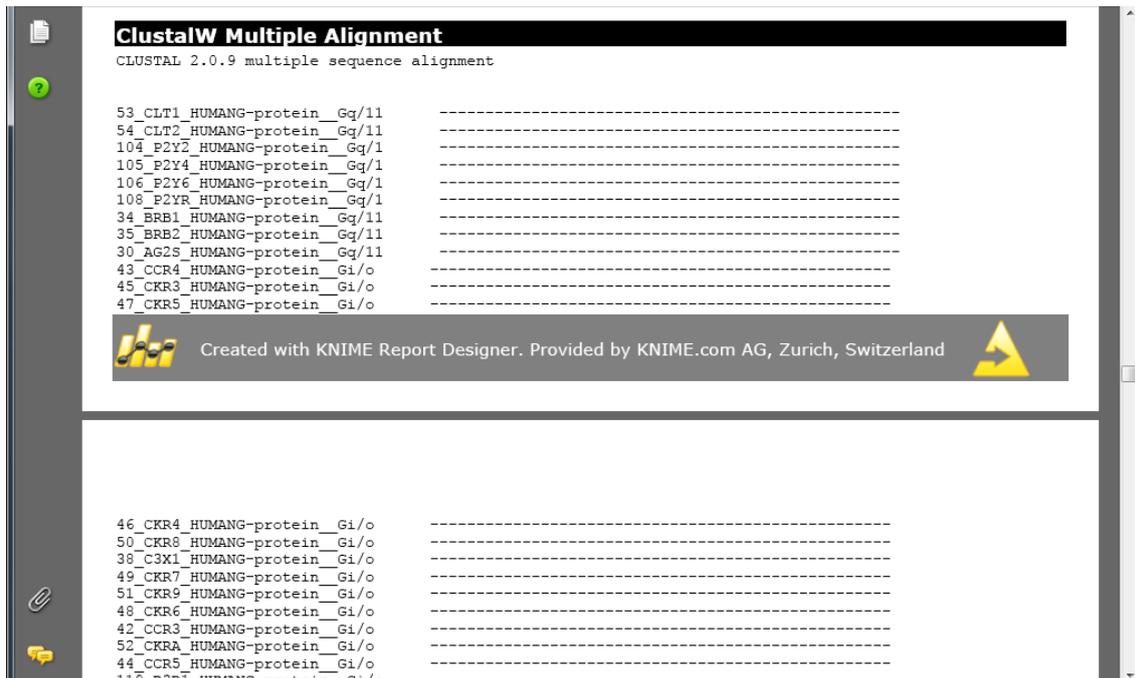
MAFFT Multiple Alignment
CLUSTAL format alignment by MAFFT FFT-NS-2 (v6.717b)

1	5H1A_HUMAN	----	M-----
2	5H1B_HUMAN	----	M-----
3	5H1D_HUMAN	----	M-----
4	5H1E_HUMAN	----	M-----
5	5H1F_HUMAN	----	M-----
6	5H2A_HUMAN	----	M-----
7	5H2B_HUMAN	----	M-----
8	5H2C_HUMAN	----	M-----
9	5H4_HUMAN	----	M-----
10	5H6_HUMAN	----	M-----
11	5H7_HUMAN	----	M-----
12	A1A_HUMAN	----	M-----
13	A1AB_HUMAN	----	M-----
14	A1AD_HUMAN	----	M-----
15	A2AA_HUMAN	----	M-----
16	A2AB_HUMAN	----	M-----
17	A2AC_HUMAN	----	M-----
18	AA1R_HUMAN	----	M-----
19	AA2A_HUMAN	----	M-----
20	AA2B_HUMAN	----	M-----
21	AA3R_HUMAN	----	M-----
22	ACM1_HUMAN	----	M-----
23	ACM2_HUMAN	----	M-----
24	ACM3_HUMAN	----	M-----
25	ACM4_HUMAN	----	M-----
26	ACM5_HUMAN	----	M-----

MAFFT Phylogenetic Tree

The phylogenetic tree is a horizontal dendrogram where the root is on the left and branches extend to the right. The terminal taxa are labeled with their IDs and names, such as 1_5H1A_HUMAN, 3_5H1D_HUMAN, 6_5H1F_HUMAN, 10_5H4_HUMAN, 17_A2AC_HUMAN, 21_AA3R_HUMAN, 23_ACM2_HUMAN, 24_ACM3_HUMAN, 25_ACM4_HUMAN, 26_ACM5_HUMAN, 27_ACTR_HUMAN, and 31_MCAR_HUMAN.

Created with KNIME Report Designer. Provided by KNIME.com AG, Zurich, Switzerland



1-9 The KNIME report contained the results of the workflow

The reporting contains the results of the workflow as follows:

- A multiple alignment generated by Mafft
- A phylogenetic tree calculated based on the multiple alignment by Mafft
- A multiple alignment generated by ClustalW
- A phylogenetic tree calculated based on the multiple alignment by ClustalW

Please let me know if you have any questions.

workflow@molprof.jp

Molecular Profiling Research Center for Drug Discovery (MolProf), AIST plans to listen to user's requests positively, and to make the system better.

Molecular Profiling Research Center for Drug Discovery (MolProf)

Advanced Industrial Science and Technology (AIST)

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