



KNIME Product Portfolio

KNIME.com GmbH, Zurich, Switzerland

The KNIME Platform



The screenshot displays the KNIME platform interface with a workflow and several data visualization windows.

Workflow: The workflow starts with a **File Reader** node (Read NCI), followed by a **Row Filter** node (Outlier), a **Domain Calculator** node (Node 47), and a **Color Manager** node (Color by class). The workflow then branches into two parallel paths. The top path includes a **Prepare NG** node, a **MetaNode 1:1** node (Node 35), and a **Parallel Coordinates** node. The bottom path includes a **MoSS** node (Node 59), a **Column Filter** node (Node 94), and another **MetaNode 1:1** node (Node 88). Both paths converge into a **Neighborhood Visualizer** node (Node 82).

Scatter Plot (#49) - Scatterplot: A scatter plot showing data points colored by class. The X-axis ranges from 100.0 to 940.0, and the Y-axis ranges from 27 to 391.

File Reader Node Description: This node can be used to read data from an ASCII file or URL location. It can be configured to read in various formats. When you open the node's configuration dialog and provide a filename, it will try to guess the reader's settings by analyzing the beginning of the file. Check the results of these settings in the preview table. If the data shown is not correct or an error is reported, you can adjust the settings manually (see below). When the node is executed it reads in the entire file and caches it in a temporary file for faster access by the connected successor nodes. It also stores all possible values it came across for each column.

Dialog Options: ASCII file location: Enter a valid file name or URL. When you press ENTER, the file is analyzed and the settings pre-set.

Interactive Table (#87) - Table View (58 x 7): A table showing chemical structures and associated data.

Key	Smiles	D Support in Focus (rel):	D Support in Complement (rel):	Atom Num:	Box
0	<chem>N#CC1=NC(=O)NC(=O)C1</chem>	14.42%	0.02%	19	20
1	<chem>N#CC1=NC(=O)NC(=O)C1</chem>	14.42%	0.03%	18	19

Interactive Table (#88) - Table View (51 x 2): A table showing chemical structures and associated data.

Key	Smiles	S Class
624486	<chem>N#CC1=NC(=O)NC(=O)C1</chem>	Cl
624487	<chem>N#CC1=NC(=O)NC(=O)C1</chem>	Cl
633772	<chem>N#CC1=NC(=O)NC(=O)C1</chem>	Cl

Neighborhood Visualizer (#82) - Interactive Neighbors: A visualization showing the neighborhood of a selected node. The X-axis is labeled 'Unity FP', 'Atompar FP', and 'VolSurf'. The Y-axis shows keys: 654633, 654826, 654995, 654956, 654967.

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Support and Maintenance Subscription





- Available for both - KNIME Desktop and KNIME Report Designer
- No functional difference between open source version
- One year subscription
 - Support requests packages
 - Standard packages for 1, 10 and 50 users and custom
 - Regular software updates
 - Patches, bug fixes and security updates between open source releases
 - Continuous access to source code
 - Local support provided by partners
 - Covering Europe, US, Japan, Asia

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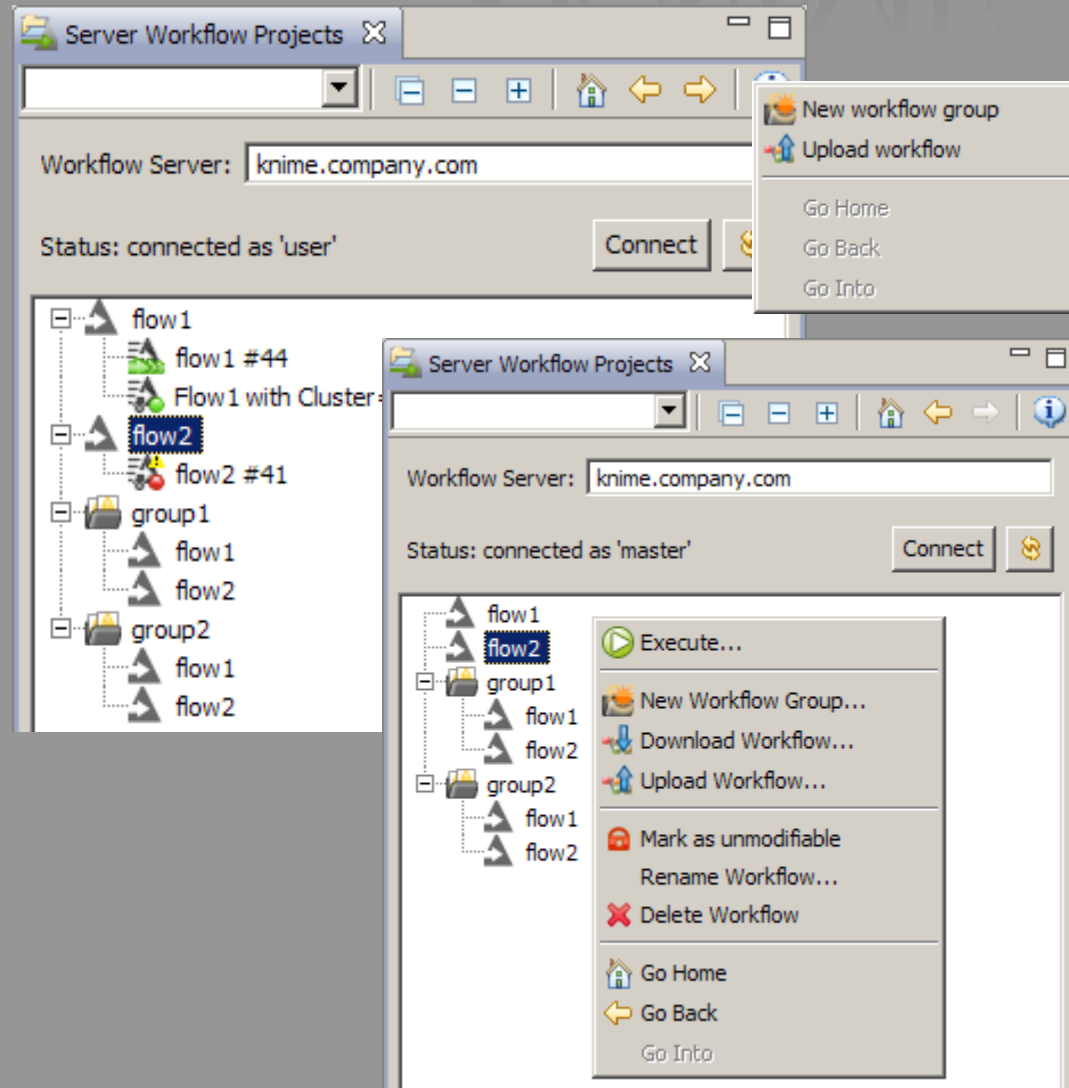
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Enterprise Server



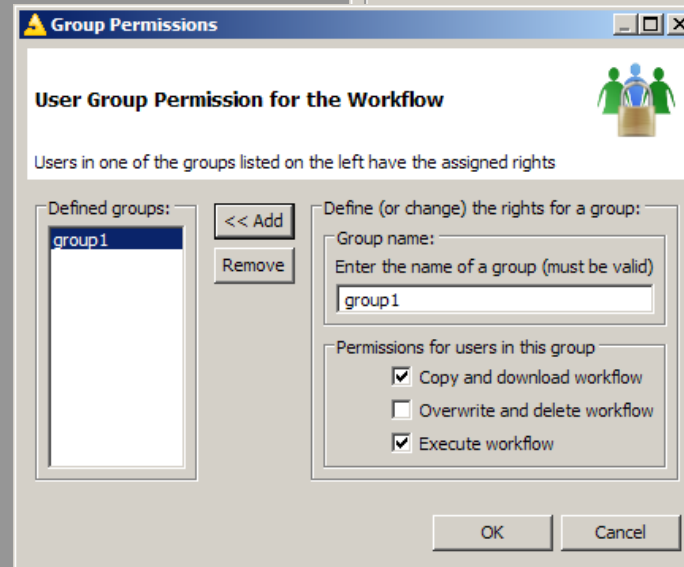
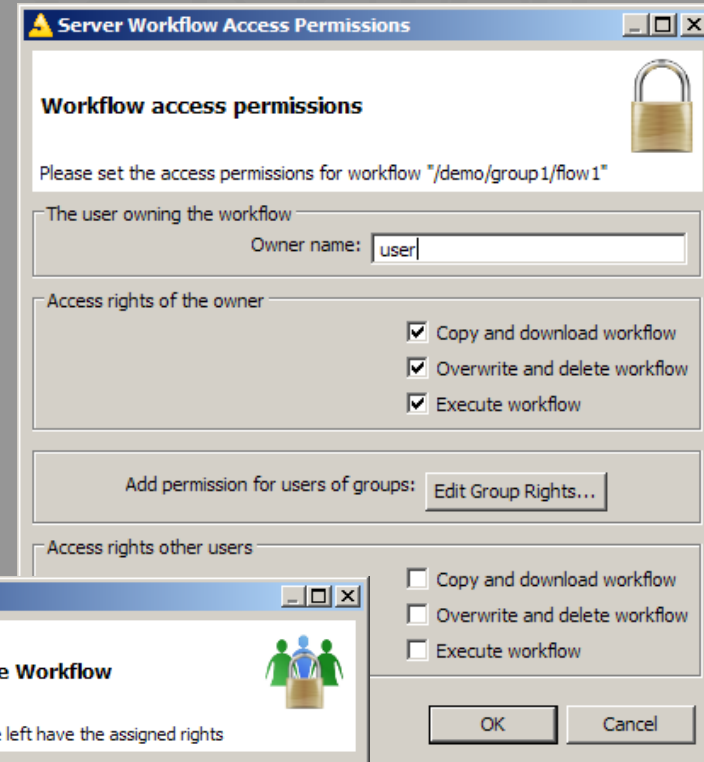
- Central shared workflow repository
- Up/download workflows
- Workflow groups for easier organization of repository



User Rights Management



- Controlled access to workflows
- Defined users and groups
- Permissions on workflows can be granted from one user to another user



Remote Execution



- Workflows can be remotely executed
- Variables can be prompted
- From workflows different jobs are created for different user
- Manual execution or scheduled for repeating tasks

- Access via
- Web Services possible

Workflow Variable Administration dialog box showing a table with columns Name, Type, and Value. The table contains one row: clusters, INTEGER, 5. There is an Edit button and an OK button.

Name	Type	Value
clusters	INTEGER	5



KNIME project tree showing a hierarchy of folders and files. The tree includes: Generated Data, Generated Data #1, Generated Data (scheduled), Generated Data (scheduled), Generated Data (scheduled), KNIME_project, Lipinski and other properties #55, LongRunningDataGern, and MasterKey2.

Server Execution Options dialog box. It includes a checkbox for 'Execute Workflow on Server', options for 'Reset before Execution' and 'Discard Workflow Job after Execution', a text field for 'Name of Workflow Job' (containing 'flow2'), a 'Master Key' field, a 'Schedule execution' checkbox, a calendar for scheduling (showing 'Mai 2010' with dates 21 and 23 highlighted), a 'Time' field (set to 23:00), and a 'Repeat every' field (set to 7 days). There are OK and Cancel buttons at the bottom.

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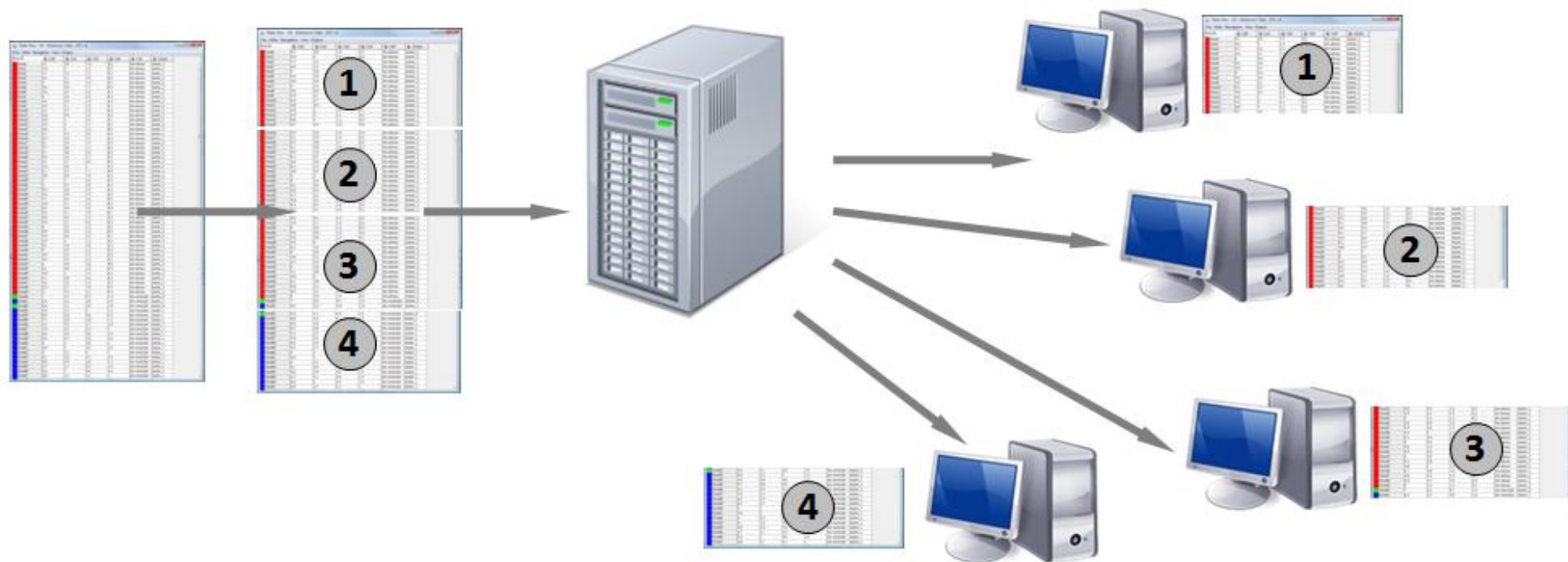
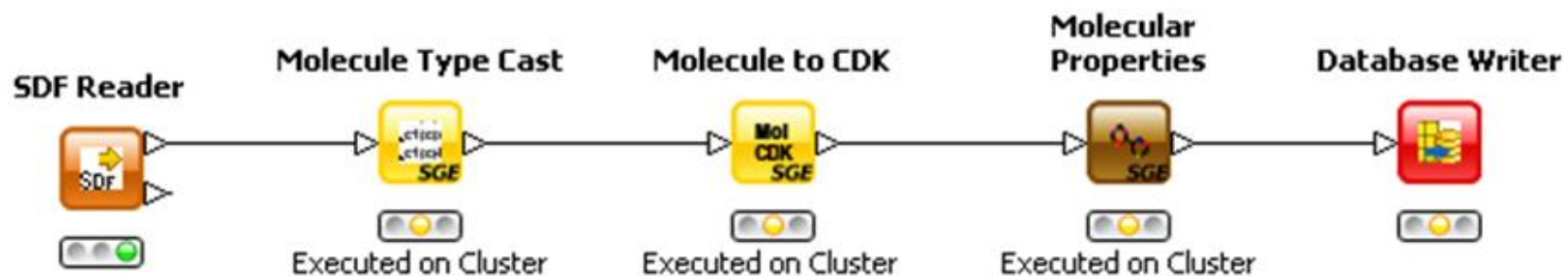
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KNIME Cluster Execution



Advantages of running workflows in a Cluster environment



Performance

- KNIME workflows can be split and executed on different resources in parallel
- For branched workflows, complete nodes can be executed in parallel on dedicated resources

Transparency of the execution

- For the end user the usage of the cluster is as simple as running workflows with the desktop version
- Allows partner nodes like ChemAxon to be executed in a grid environment





ChemAxon nodes run in a Cluster environment

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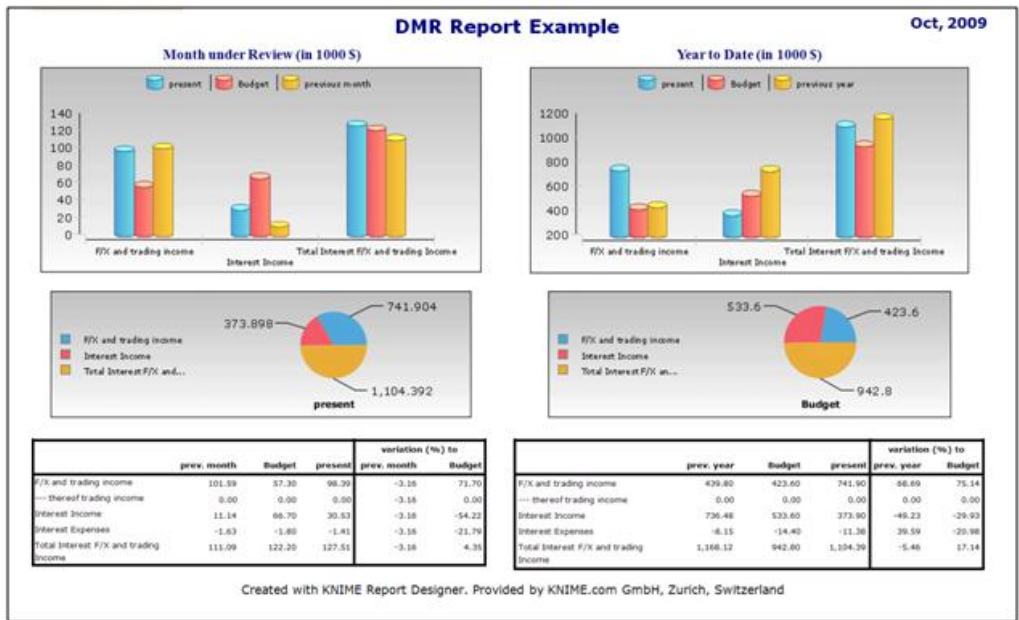
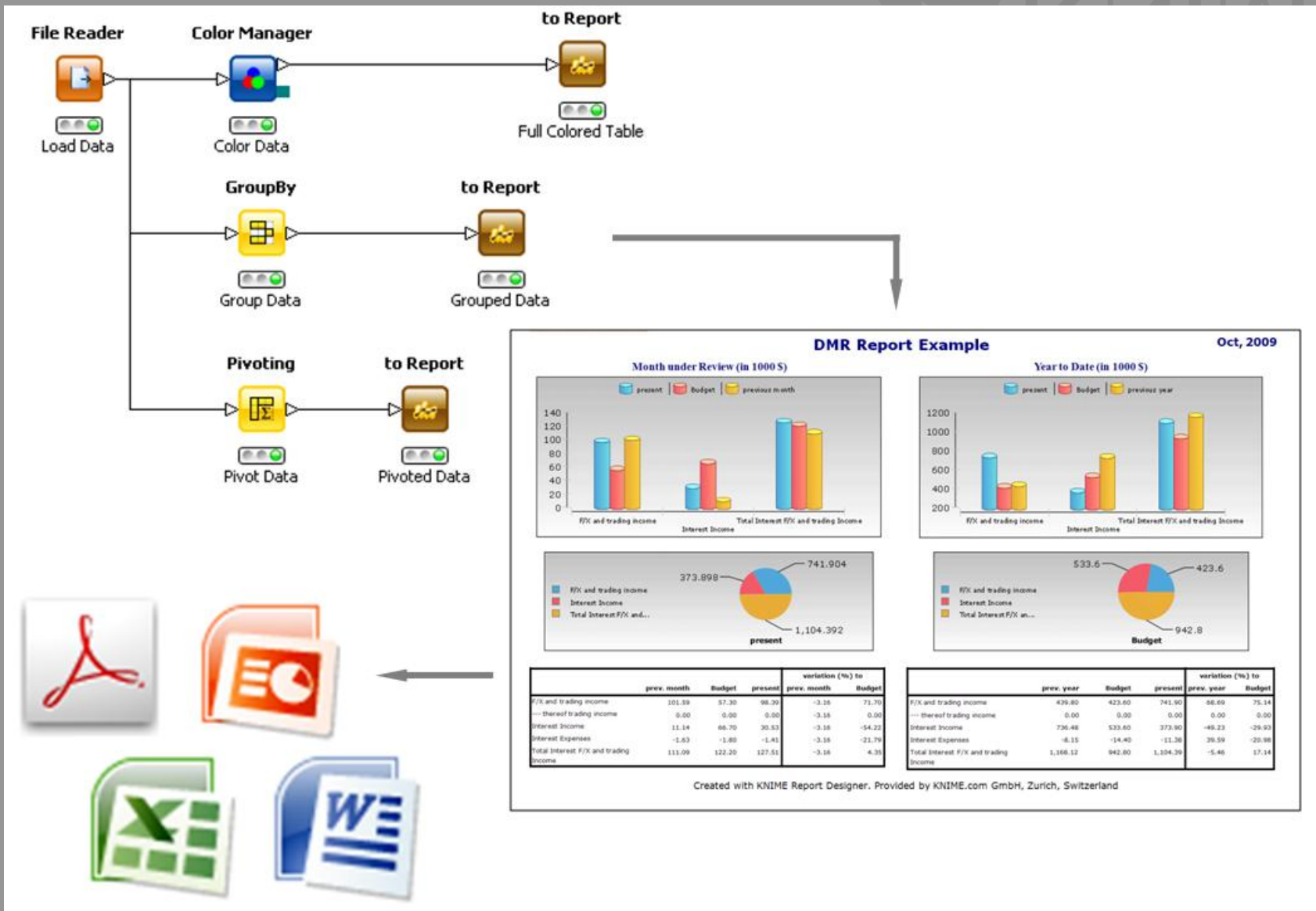
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KNIME Report Designer



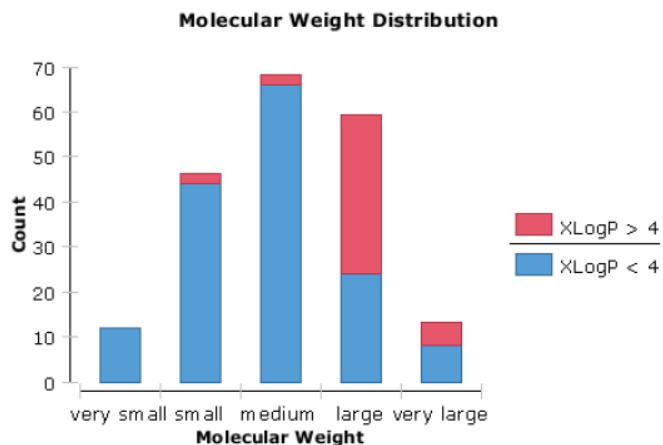
KNIME Report Example

Final Report



SAR example

Created on NCI Data Set, table shows 5 selected structures.

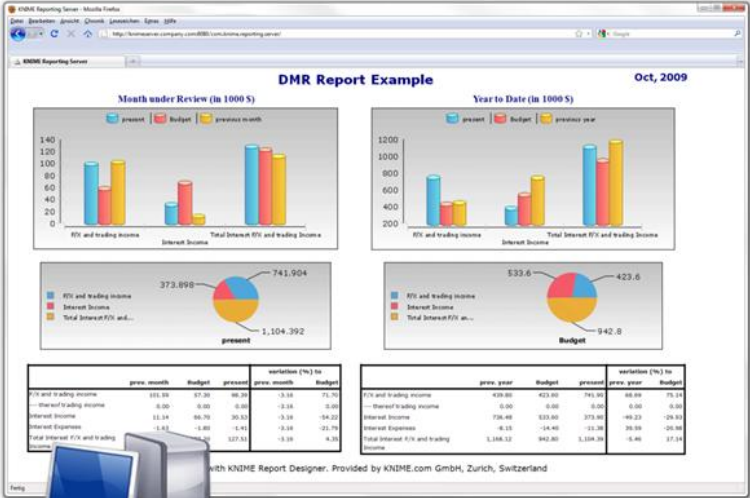
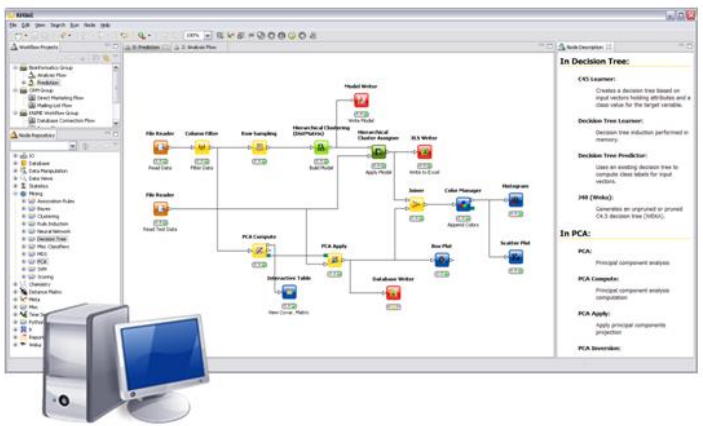
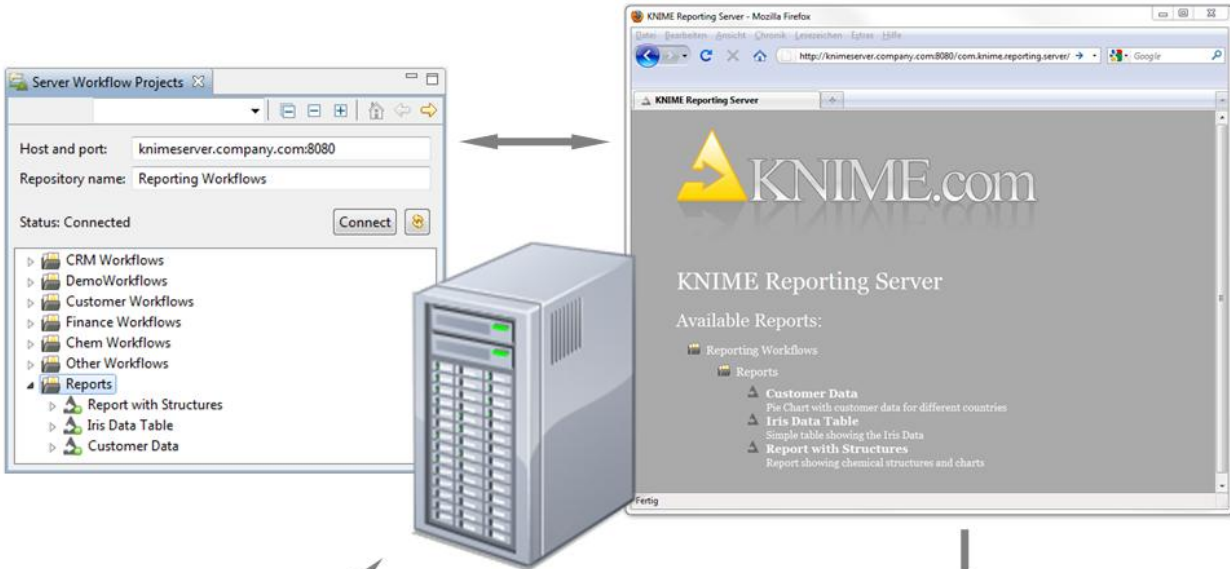


Molecular Weight	xlogp < 4	xlogp >= 4
very small	12	0
small	44	2
medium	66	2
large	24	35
very large	8	5

NSC	Molecule	XLogP	Mol. Weight
89	 <chem>CN(C)CC(=O)c1ccccc1</chem> HCl	2.09	213.09
171	 <chem>O=C(O)c1cccnc1</chem>	-1.69	123.03
185	 <chem>Oc1c(O)c2c(O)c(O)c(O)c2c1</chem>	0.76	281.16
186	 <chem>Cc1c(O)c(O)c(O)c(O)c1</chem>	1.62	250.08
291	 <chem>O=C1N(C(=O)O1)c2ccccc2</chem>	3.78	249.08



KNIME Report Server



with KNIME Report Designer. Provided by KNIME.com GmbH, Zurich, Switzerland

KNIME Reporting



- Provides access to KNIME workflows without exposing the underlying workflows and nodes
- Templates created by an expert
- End users just execute the template and export the data to the desired format

KNIME Services



KNIME Training

End User and Developer Training

KNIME Consulting Services

KNIME Custom Development Services

- Schrödinger
- Symyx Technologies
- Tripos
- CambridgeSoft
- ChemAxon / Infocom
- Molecular Discovery
- Trewaren
- Spotfire
- BioSolve IT

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CCG (Chemical Computing Group)



Thank You



For more information:

info@KNIME.com

<http://www.KNIME.com>

KNIME.com GmbH

Technoparkstr.1

8005 Zurich

Switzerland

Tel: +41-44-445-2660

Fax: +41-44-445-2662

