



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 main workflow consists of the following nodes: File Reader (Read NCI) → Row Filter (Outlier) → Domain Calculator (Node 47) → Color Manager (Color by class) → Prepare NG → MetaNode 1:1 (Node 35) → MoSS (Node 59) → Column Filter (Node 94) → Interactive Table (Node 87) → Interactive Table (Node 88) → Neighbor → Parallel Coordinates → Scatter Plot (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):

File	Hilite	Navigation	View	Output		
Key	smiles	D Support in Focus (rel):	D Support in Complement (rel):	Atom Num:	Is	Box
0	<chem>N#Nc1ccc(O)c2c1O</chem>	14.42%	0.02%	19	20	
1	<chem>O=C1NC(=O)NC1=O</chem>	14.42%	0.03%	18	19	

Interactive Table (#88) - Table View (51 x 2):

File	Hilite	Navigation	View	Output
Key	smiles	S	Class	
624496	<chem>N#Nc1ccc(O)c2c1O</chem>		Cl	
624487	<chem>N#Nc1ccc(O)c2c1O</chem>		Cl	
633772	<chem>N#Nc1ccc(O)c2c1O</chem>		Cl	

Neighborhood Visualizer (#82) - Interactive Neighborhoods:

File	View	Hilite	Hide	Fade	Cluster
Key	Unity FP	Atompar FP	VolSurf		ClusterQuality
654633					
654826					
654995					
654956					
654967					

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KNIME Server Lite		
 KNIME Report Server	 KNIME Enterprise Server	 KNIME Cluster Execution

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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 contract
 - Support requests packages
 - Standard packages for 1, 10 and 50 users
 - Custom packages are available
 - Regular software updates
 - Patches, bug fixes and security updates between open source releases
 - Continuous access to source code
 - Assigned support representative at KNIME.com
 - Discounted one day KNIME training at KNIME.com in Zürich

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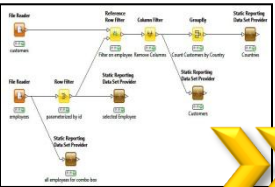
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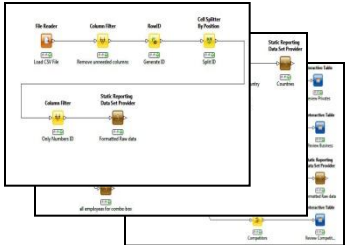
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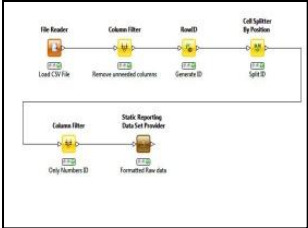
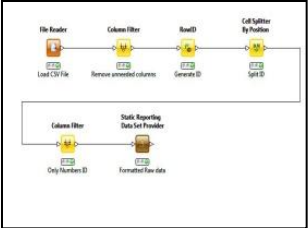
KNIME Server Lite



Remote Execution



Shared Workflow Repository



Concept behind Server Lite

Provides basic workgroup capabilities

- Remote workflow repository
- Upload and download of workflows
- Remote execution

Usage of Server Lite



Workgroups



- Exchange workflows between group members
- Execution of calculation intensive workflows

- No need for user access right management
- No need for version control

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Time Line



First preliminary version (available now for internal use)

- User rights management
- Workflow execution
- Shared workflow repository



Version 1 (mid 2010)

- Scheduled execution
- Web services
- Meta Node repository

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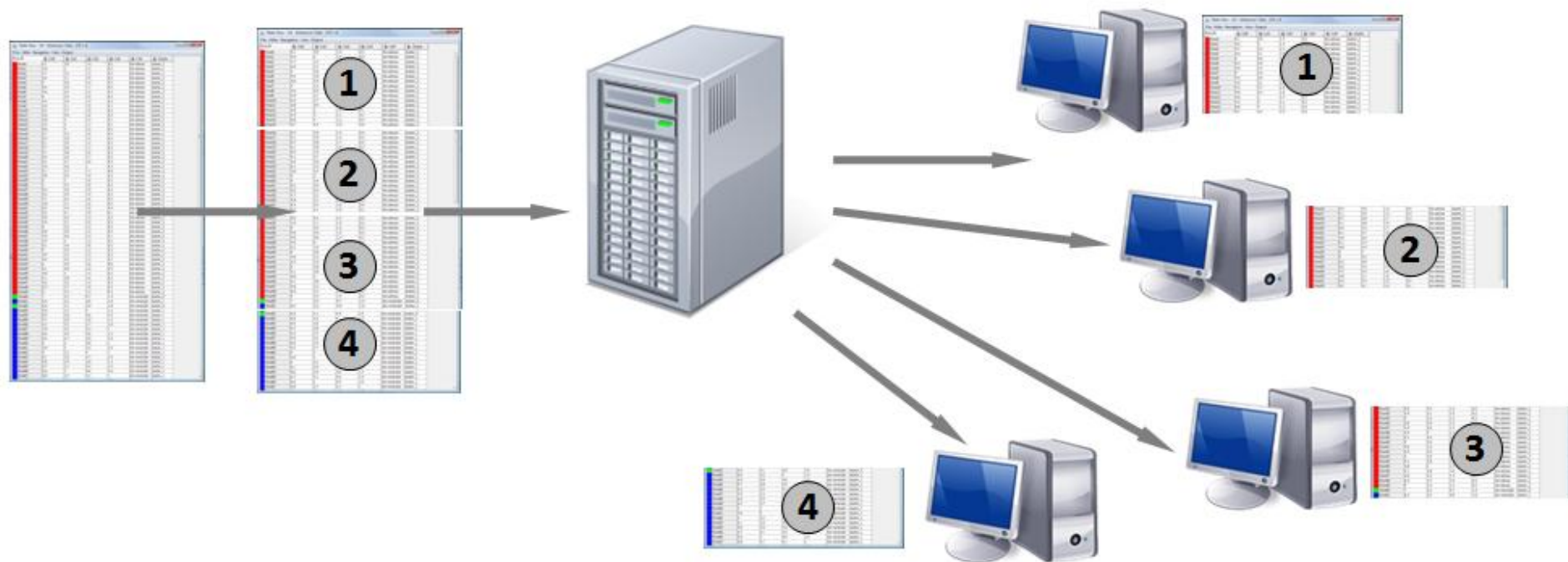
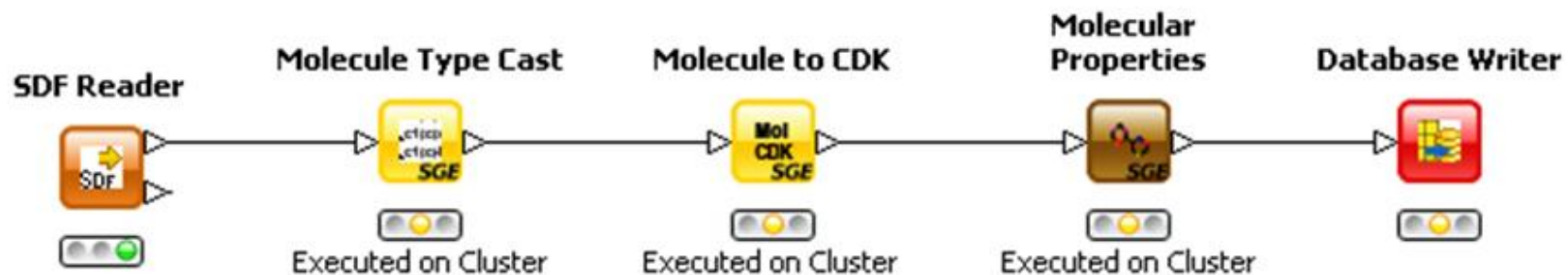
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KNIME Cluster Execution Task Splitting



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

Remote execution

- Allows the submission of a workflow and disconnection of the client
- After the workflow is completed the user can reconnect and the results can be downloaded



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 to be executed in a grid environment


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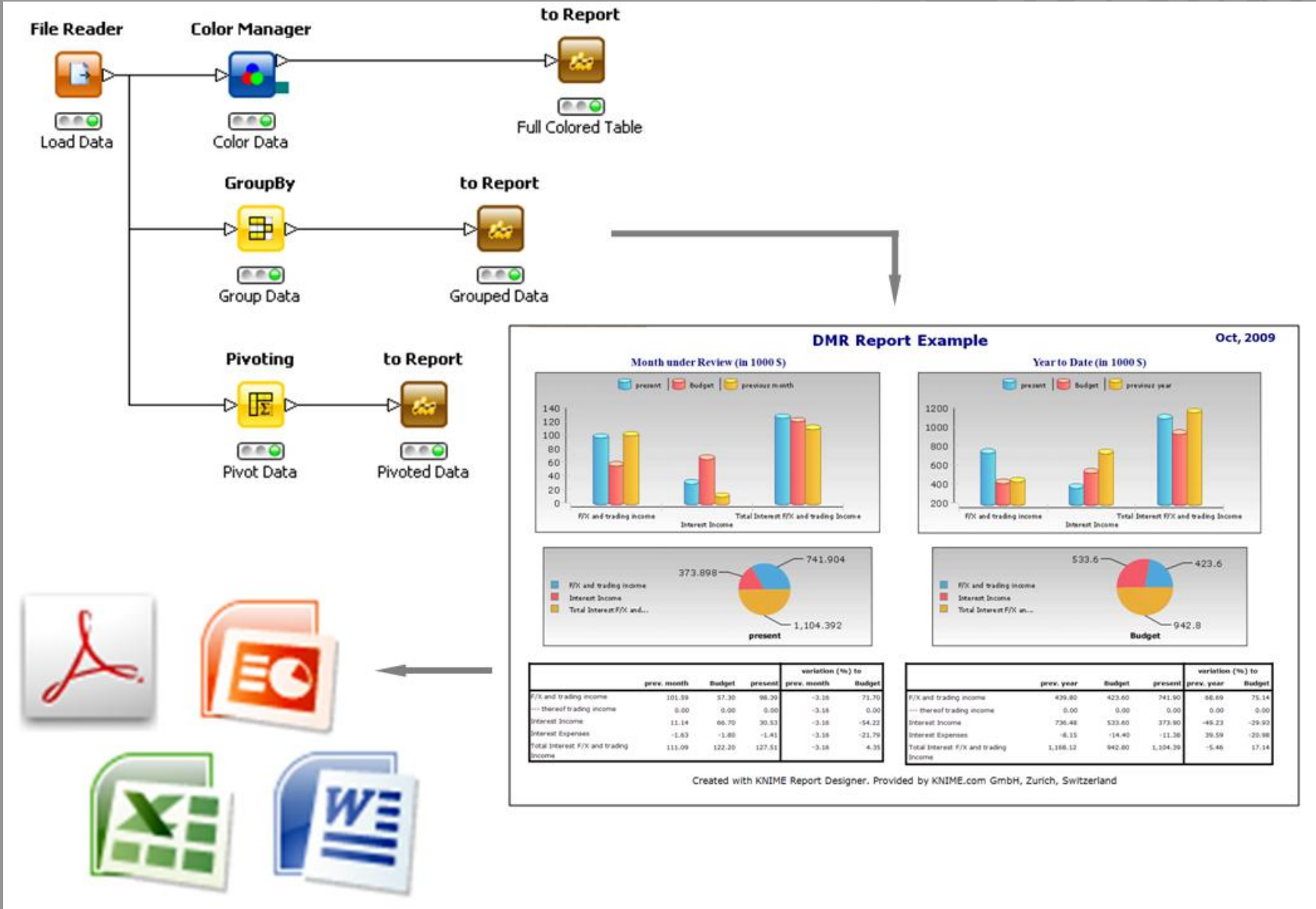
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KNIME Report Designer



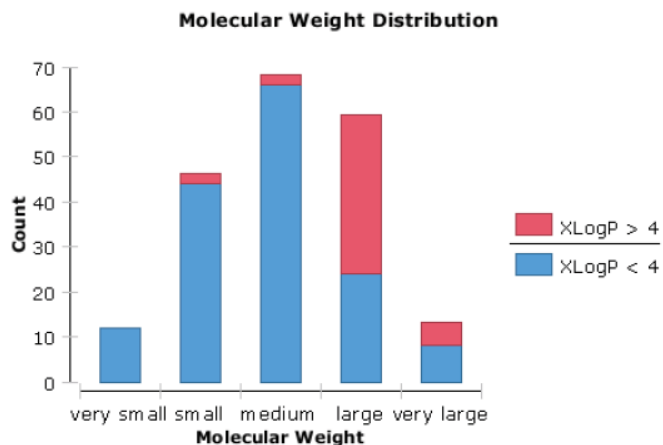
KNIME Report Example

Final Report



SAR example

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

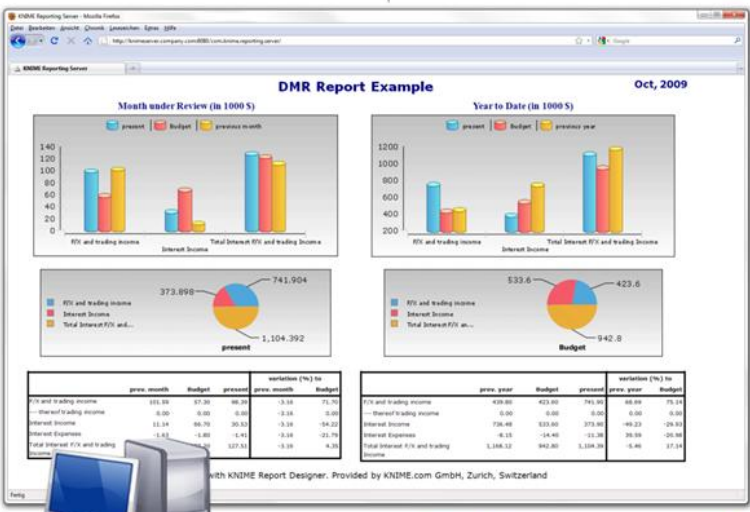
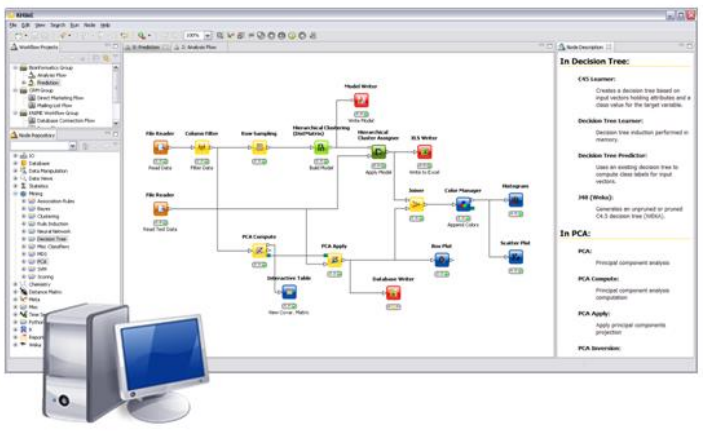


Molecular Weight	xlogp < 4	xlogp >= 4
very small	12	0
small	44	2
medium	66	2
large	24	35
very large	8	5

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>C[C@H]1[C@@H](C)[C@H](O)[C@@H](C)C(=O)N1C(=O)C</chem>	0.76	281.16
186	 <chem>COC1=CC(=C(C=C1)C(=O)O)C(=O)O</chem>	1.62	250.08
291	 <chem>O=C1NC(=O)C=C1c2ccccc2</chem>	3.78	249.08



KNIME Report Server



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

Thank You



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