

Schrödinger extensions

- **150+ nodes:**
 - Covering most of the Schrödinger tools
 - Most recent additions: Residue scanning, Prime Energy, SiteMap, PyMOL, Glide grid writer
 - Many take in and output sdf and pdb or mol2 on top of Maestro format
 - Newest nodes use the same configuration panel as Maestro (see the Residue scanning node)
 - Structure and data manipulation nodes (eg Split by structure, delete atoms)
 - GUI nodes (eg Run Maestro, Run PyMOL)
 - Scripting nodes: Run Maestro command, Chemistry external tool, Python nodes
 - Utility nodes: Setup diagnosis and workflow list
- **50+ workflow examples**
 - Workflow page: descriptions and download the ones of interest
 - Whole set can be downloaded with the Suite
 - Many other workflow drafts available on demand

Schrödinger extensions

- Tested with latest KNIME version and include the version available at the time of the release
- Parameter flow variable capability
 - Use the options not exposed in the configuration panels (eg command line only)
 - Implemented for the main nodes eg Glide, MMod (eg OPLS 2.1), Jaguar
- 2D renderer
 - 2D coordinate generation and rendering
 - The default renderer can be set for Maestro columns
 - Can be used in the Report designer

Schrödinger extensions

- More and simplified start-up options and stand-alone installation configuration in the Preferences
 - In `$SCHRODINGER/knime` start-up script
 - eg use a stand-alone KNIME installation, set temporary directories, the memory limit...
- KNIME menu in Maestro
 - Connect to KNIME mode to exchange structures with a KNIME session
 - KNIME-Maestro connector node (Improved in 2015-1: automatic connection/close, more modes)
 - Build, import, edit and run workflows from Maestro on project table data
 - Dynamically generated GUI to alter some parameters.
- Simplified batch execution: `KNIME_batch.py`
 - Batch command generation based on workflow annotations
 - Stand-alone dynamically generated GUI
 - Useful options eg `-stderr/out`
- Easier installation creation and update
 - Using Eclipse machinery in `KNIME_install.py`
 - eg list of extensions to install, from several (zipped) update sites

Schrödinger extensions

See details in:

http://www.schrodinger.com/upload/KNIME_Overview.pdf

- **The new features slides:**
 - Parameter flow variables (2014-1)
 - Simplified batch execution (2013, 2014-1)
 - Chemistry external tool node improvements
 - KNIME menu in Maestro (2012)
 - Start-up script (2012)
- **Workflow examples:**
 - Labs > Parameter flow variable usage
 - General > Installation (KNIME_install.py scenarios)
 - General > Workflow list
 - General > Chemistry external tool node usage
 - Phase > Shape screening, docking (batch execution)
 - 2D renderer in the report designer

Why use KNIME

Automation

- Automate repetitive tasks (especially complex / error prone tasks)
 - e.g. PDB set preparation, Ligand database preparation

Collaboration

- Share workflows with colleagues (also in Maestro and Seurat)
- Not a black box
 - e.g. Ensemble docking, HTS analysis

Prototyping

- Test parameters
 - e.g. Validate docking parameters

Documentation

- Easy debugging, interruptions, data included, inspect each step (2D, in Maestro/PyMOL)

Combine various Tools

- Schrodinger and third party tools (vendor agnostic), scripts (Python, Java, shell),
 - e.g. QM workflows

Reporting

- Nodes for reporting results
 - e.g. Enrichment plotter node, pdf, tables, etc.
- KNIME report designer (free), web portal (KNIME.com)

Inexpensive

- Organized by level:
 - Get started
 - Intermediate
 - Advanced functionalities
- And by topics:
 - KNIME desktop: GUI, specificities, nodes
 - Schrödinger extensions: specificities, nodes
- You can jump between the sections using links (marked with ► or ◀). See the overview slides.
- There are also links to use-case examples (marked with ♦).

Get started

KNIME desktop

- GUI
- Specificities
- Nodes

Schrödinger extensions

- Specificities
- Schrödinger nodes



Intermediate



- Knime.org and Knime.com
- KNIME desktop
- Start Knime
- Create a new workflow and organize a workspace
- Run a node
- Import and export workflows
- Tips and tricks
- Documentation

KNIME Extensions

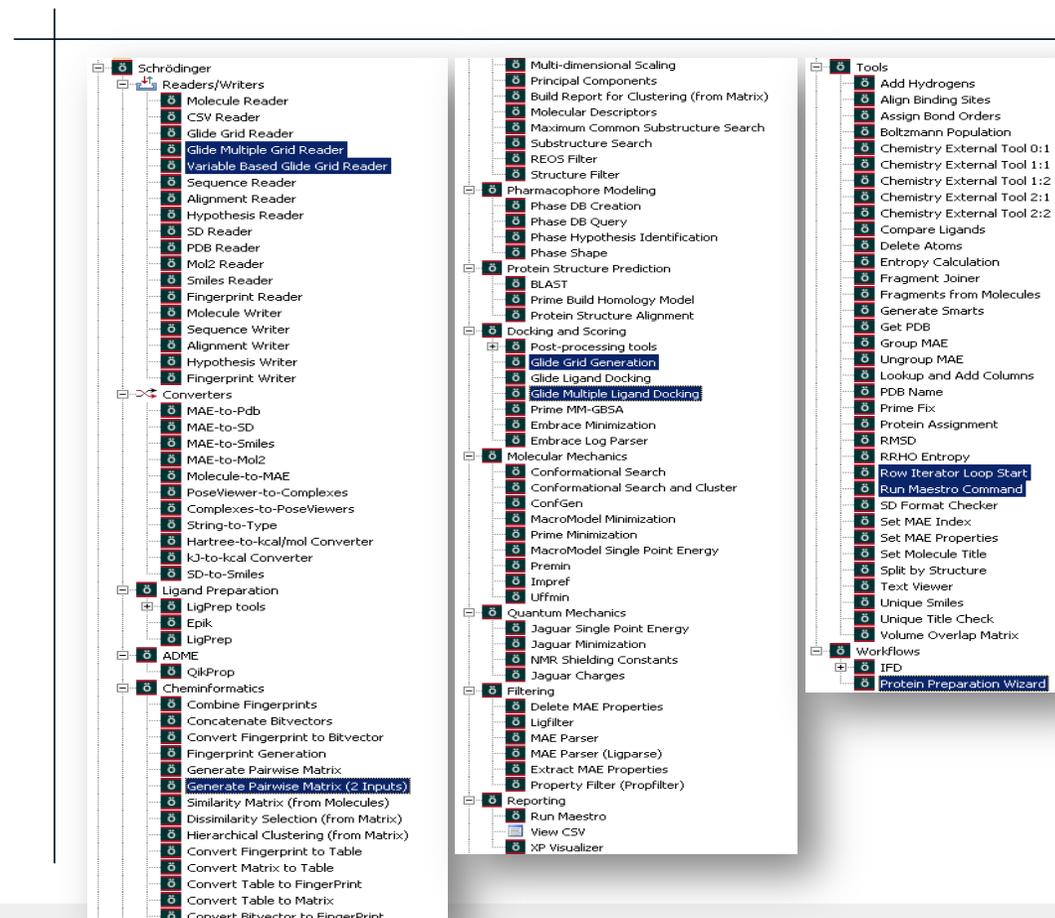
15+ Extension Providers

Extensible, cross-platform, vendor neutral:

Schrödinger, CCG, Tripos, ChemAxon/Infocom, BioSolveIT, Cresset, Dotmatics, Molecular Discovery, Molegro...

Schrödinger Extensions

- First released in 2007
- 150+ nodes
 - Molecular mechanics
 - Molecular dynamics
 - Quantum mechanics
 - Cheminformatics
 - Pharmacophore modeling
 - Combinatorial libraries
 - Docking
 - Protein structure prediction
 - Structure and data manipulation
- Maestro integration
 - Workflow execution
 - Structure exchange



KNIME Desktop GUI

The screenshot displays the KNIME Desktop GUI interface. Key components are highlighted with red circles:

- Workflow Projects:** A list of saved workflow projects on the left side.
- Node Repository:** A tree view of available nodes, with 'Phase Shape' selected under 'Pharmacophore Modeling'.
- Workflow Canvas:** A central workspace showing a workflow with nodes like 'Molecule Reader', 'Phase Shape', 'Extract MAE Properties', 'Sorter', and 'GroupBy'.
- Node Description Panel:** A right-hand panel showing the 'Phase Shape' node's documentation, including its purpose, backend implementation, dialog options, and output column structure.
- Console:** A bottom panel displaying system logs and execution messages.

- Full screen mode
- Forget about Eclipse specific menu items

More about:

- The console ▶

Start KNIME

- Start up KNIME:
 - On Linux: run `$SCHRODINGER/knime`
 - On Windows: click on the icon
 - Use `-data MyWorkspace` to open a specific workspace
 - File > Switch workspace, but KNIME takes time to start up again
- Workspace, workflows and workflow groups:

The screenshot displays the KNIME software interface. The top menu bar includes File, Edit, View, Search, Run, Node, and Help. Below the menu is a toolbar with various icons for file operations and workflow management. The left sidebar shows a tree view of 'Workflow Projects' with a list of workflow groups and nodes under 'Cheminformatics'. The main workspace shows a workflow diagram with the following nodes and data:

- Smiles Reader**: Input is '1312 ASDI fragments (.smi)'. It has a warning icon and a green status indicator.
- Fingerprint Generation**: Output is 'Linear (Daylight) fingerprint'. It has a green status indicator.
- Generate Pairwise Matrix**: Output is 'Tanimoto metric'. It has a green status indicator.
- Build Report Clustering (**: Output is 'Analyze differe...'. It has a green status indicator.

```
graph LR; A[Smiles Reader] --> B[Fingerprint Generation]; B --> C[Generate Pairwise Matrix]; C --> D[Build Report Clustering];
```

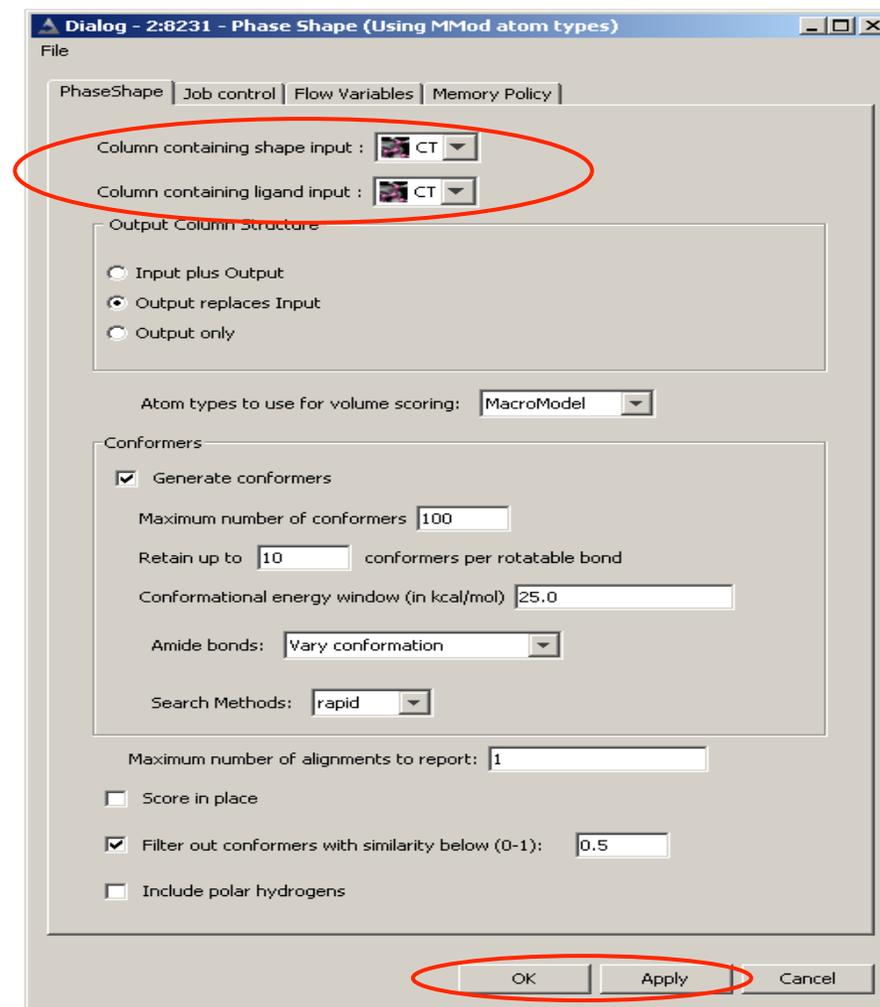
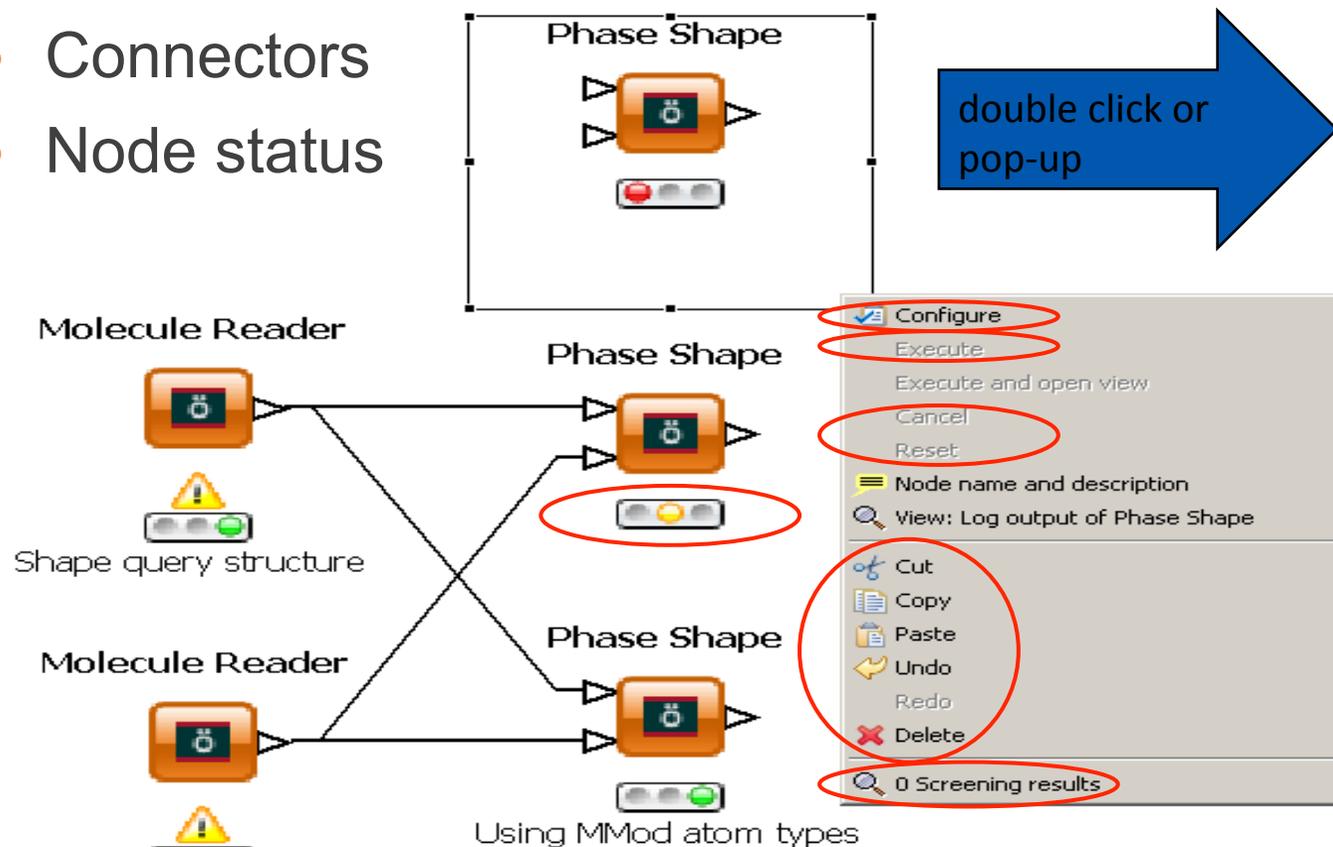
Create a new workflow and organize a workspace

- Under the pop-up menu of Workflow Project repository:
 - New KNIME workflow and New Workflow group
 - Copy, Paste, Delete, Move, Rename
- Drag and drop the workflows in the Workflow project repository

The screenshot displays the KNIME software interface. The top menu bar includes File, Edit, View, Search, Run, Node, and Help. Below the menu is a toolbar with various icons for file operations and workflow management. The main workspace is divided into two panes. The left pane, titled 'Workflow Projects', shows a hierarchical tree structure of workflow projects. The right pane shows a context menu with options: New KNIME workflow..., New Workflow Group..., Open, Copy, Paste, Delete, Move..., Rename..., Import KNIME, Export KNIME, Workflow Variables, Configure..., Execute..., Cancel Execution, Reset, and Edit Meta Information. A 'New KNIME Workflow Wizard' dialog box is open in the foreground, prompting the user to create a new workflow. The dialog has a title bar with the KNIME logo and a close button. The main text reads 'Create a new KNIME workflow.' Below this, there are two input fields: 'Name of the workflow to create:' with the text '<KNIME_project' and 'Workspace destination:' with the text '/Examples/Cheminformatics' and a 'Browse...' button. At the bottom of the dialog are 'Finish' and 'Cancel' buttons.

Run a node

- Connectors
- Node status



LigPrepped structures to screen

- Input and output data tables

Screening results - 2:8222 - Phase Shape (Using MMod...)

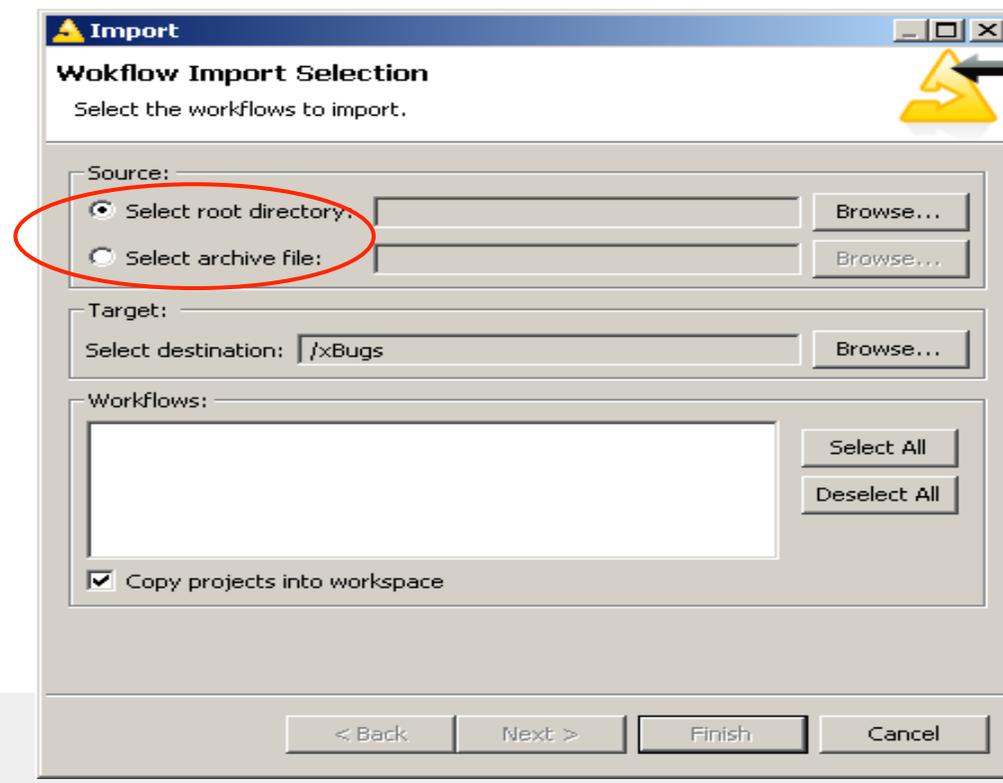
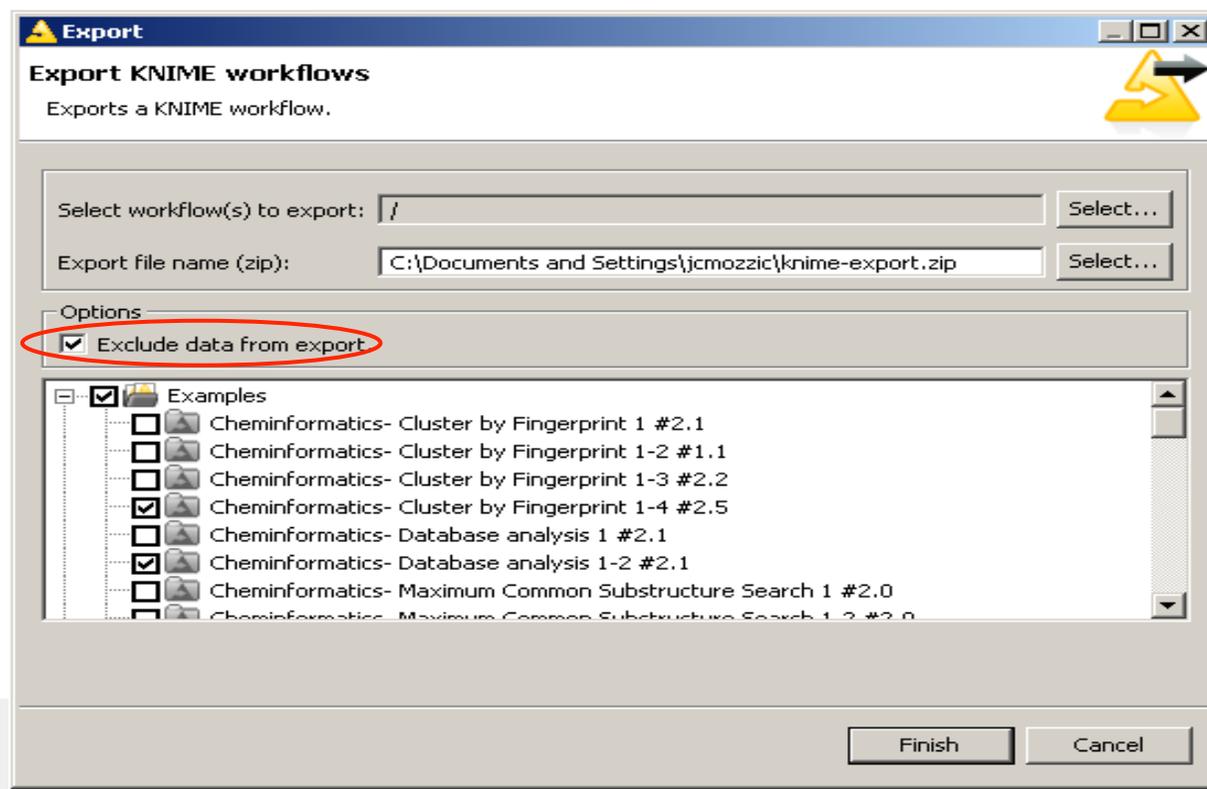
File

Table "default" - Rows: 26 | Spec - Column: 1 | Properties | Flow Variables

Row ID	CT
Row127	Molecule: 500007027 #atoms:...
Row128	Molecule: 500007029 #atoms:...
Row171	Molecule: 500008361 #atoms:...
Row220	Molecule: 500009109 #atoms:...
Row221	Molecule: 500009111 #atoms:...
Row228	Molecule: 500009129 #atoms:...
Row600	Molecule: 500015549 #atoms:...
Row612	Molecule: 500015733 #atoms:...

Import and export workflows

- File > Import KNIME workflow / Export KNIME workflow or under the pop-up menu of a Workflow Project group
- Import from another workspace or an archive file (zip)
- Select 1 or several workflows > export as a zip file
Exclude or not the cached data from the exported file



Tips and tricks

- Save regularly the changes. Since KNIME 2.10 there is an auto save functionality but it isn't on by default.
Save while running calculations (see Preferences ►)
- Multiple undo and redo apply on workflow edition (execution data lost though)
- The KNIME desktop isn't based on a client-server architecture. If you close the KNIME instance while a calculation is running it won't kill it nor you will be able to recover the results when opening the workflow again.

Documentation

- Node descriptions. Also accessible from Help > Help content > Knime > Node descriptions
Type in search field and inspect the configuration panel
- Product page <http://www.schrodinger.com/KNIME-Extensions>
New Features, New Features Slides, KNIME Overview
- Schrödinger KNIME manual `$$SCHRODINGER/docs/knime/user_manual/kni13_user_manual.pdf`
- Schrödinger FAQs <http://www.schrodinger.com/kb>
- Workflow page (examples) <http://www.schrodinger.com/knimeworkflows/>
- Schrödinger's extensions webex <http://www.schrodinger.com/seminarprior/19/24/>
- KNIME.org
 - Workflow examples (preconfigured server access in KNIME explorer)
 - Screencast <http://www.knime.com/introduction/screencasts>
 - Forum <http://www.knime.org/forum/>

- Preferences
- Advanced node functionalities
- Errors, warnings and Console information
- Flow variables and workflow variables
- Metanodes
- Memory limit
- Tips and tricks



- Stepwise execution
- Data table column types and conversion

Stepwise execution

- Only stepwise execution
Ideal to take advantage of Schrödinger's jobcontrol infrastructure
- No predefined execution order for non connected branches. Use the flow variable ports [KNIME 2.3]
- Data cached at each step
- Preferences > KNIME > Maximum working threads for all nodes
- 1:1 connection between nodes (use the concatenate node to combine input flows)

Data table column types and conversion

- KNIME relies on strict data table column typing
- Converter nodes:
 - Double to Int (integer), String to number, Number to string
 - Molecule type cast (but no Maestro conversion)
 - Openbabel, CDK to molecule, Molecule to CDK
- In the Schrödinger extensions:
 - String-to-type
 - Molecule-to-MAE, MAE-to-Pdb, MAE-to-SD, MAE-to-Smiles, MAE-to-mol2, SD-to-smiles
 - Canvas object converters

Schrödinger specific cell types

- Structures: Maestro, Sequence, Alignment
- Several files: Glide grid, Phase Hypothesis
- Desmond trajectory
- Binary formats: Canvas fingerprint and matrix

The image displays a screenshot of the Schrödinger Maestro software interface. The main window shows a table with columns: Row ID, CT, s_m_title, and activ. The CT column contains entries like 'Molecule: 1AC8 #atoms:...' and '#CTs: 2'. Two red circles highlight the CT values '1AC8' and '#CTs: 2'. Overlaid on this are several smaller windows:

- Sequences in Maestro format - 9:11 ...**: A table with columns Row ID and Sequence. Row 1 shows 'Sequence length: 298'.
- Alignments in Maestro fo...**: A table with columns Row ID and Alignment. Row 1 shows '#Alignments: 517'.
- Molecular fingerprints in Binary format - 7:44 - Finger...**: A table with columns Row ID and FingerPrint. Row 1 shows 'Fingerprint: size=1703936 bytes, 32 bit precision'.
- Pairwise distance matrix in Binary format - ...**: A table with columns Row ID and CanvasMatrix. Row 1 shows 'Canavs Matrix: size=6911626 bytes'.
- Glide Grid - 8:73 - Glide Multiple G...**: A table with columns Row ID and GlideGrid. Row 1 shows 'Grid Prefix="grid_1bl7" zipped' and Row 2 shows 'Grid Prefix="grid_1bl7_altered" zipped'.

Readers and writers, converters



- KNIME workbench nodes
- Data manipulation nodes
- Data exchange

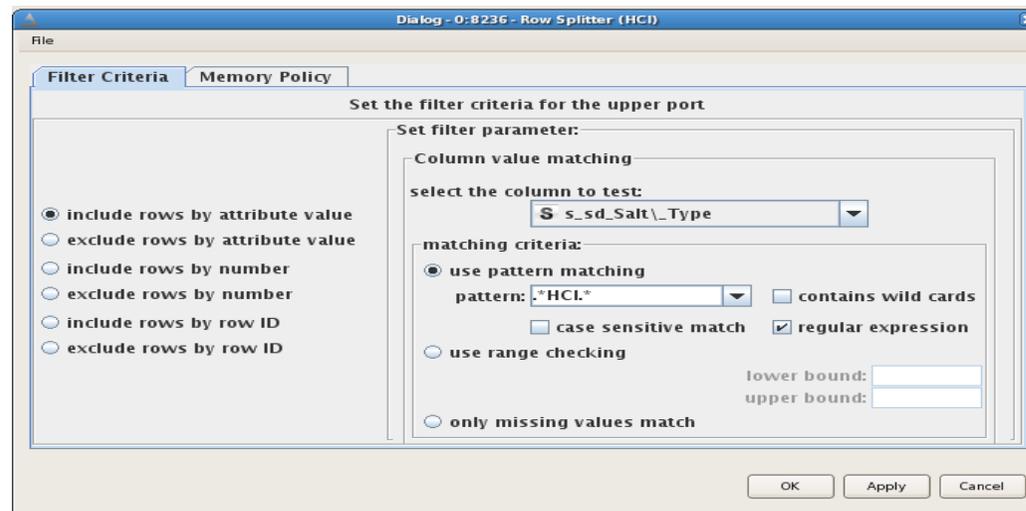
KNIME workbench nodes

+ ... 	IO
+ ... 	Database
+ ... 	Data Manipulation
+ ... 	Data Views
+ ... 	Statistics
+ ... 	Mining
+ ... 	Chemistry
+ ... 	Distance Matrix
+ ... 	Loop Support
+ ... 	Meta
+ ... 	Misc
+ ... 	KNIME Labs
+ ... 	Time Series
+ ... 	Python
+ ... 	R
+ ... 	Reporting
+ ... 	Weka

- I/O nodes for reading and writing data from files and databases
- Data manipulation nodes for managing the internal data tables that are used to pass information between nodes
- Charting and plotting tools
- Loop support, time Series, Distance matrix
- Statistics and data mining nodes (Mining, Weka) such as clustering, neural networks, decision trees, Lib SVM
R statistical computation
- Basic chemistry-aware nodes (CDK)
very limited, see Schrödinger extension nodes ►

The most often used nodes for data manipulation

- Row filter, Row splitter and Sorter
- Column filter, Column resorter, Column combiner and Rename
- Joiner (see also Schrödinger Look up and add column node ►) and Concatenate (only 2 inputs)



And also:

- Java snippet, RowID and GroupBy node ►
- Schrödinger nodes for data manipulation ►

Data exchange



- As text files: File reader and csv writer nodes
- In Excel format: xls reader and xls writer nodes
- Between workflows: table reader and table writer nodes
- See also among the Schrödinger nodes:
 - Schrödinger reader and writer nodes
 - CSV reader (read several files)
 - View CSV ▶

- KNIME.com Labs nodes
- Scripting and run a third party tool
- Java snippet
- RowID
- Group by
- Miscellaneous nodes: Interactive table, Math formula, CDK Sketcher
- Plotting facilities
- Looping functionalities - Basics
- Model building nodes



- Canvas 2D renderer
- Grouped structures in a cell
- Output column structure options
- Jobcontrol tab

Canvas 2D renderer

- Preferences > KNIME > Preferred renderer

Molecules in Maestro format - 5:41 - Mole...

File

Table "default" - Rows: 1347 | Spec - Column: 1 | Properties

Row ID	CT
Row1	 Available Renderers ▶ Maestro Molecule Summary Maestro File ● Canvas 2D String
Row2	
Row3	
Row4	
Row5	

Preferences

type filter text

- Ant
- Data Management
- General
- Help
- Install/Update
- Java
- KNIME
 - Chemistry
 - Database Driver
 - KNIME Explorer
 - KNIME GUI
 - Master Key
 - Meta Info Preferences
 - Network
 - Open Street Map
 - Perl
 - Preferred Renderers
 - Report Designer
 - Schrödinger
- Plug-in Development
- Report Design
- Run/Debug
- Team

Preferred Renderers

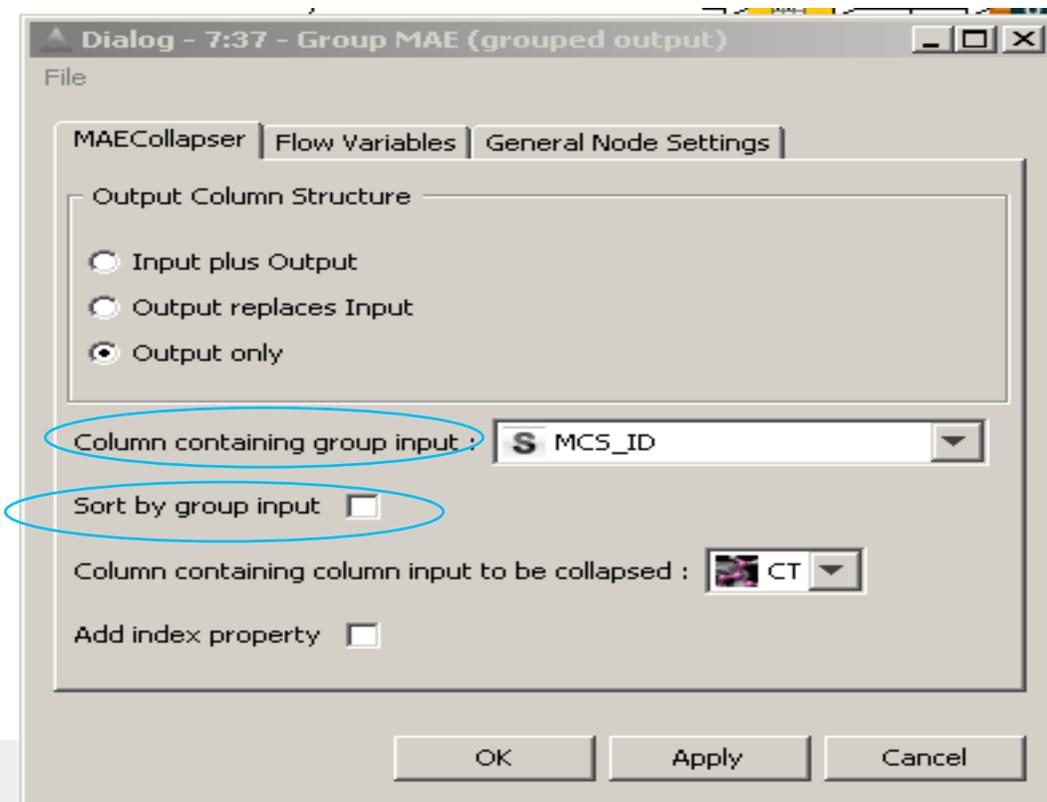
Select the preferred renderer that should be used in table view reports for any available data type. The selection for data type that have only one renderer is disabled.

- Basic
- Biology
- Chemistry
 - Maestro: Maestro Molecule Summary
 - Mol2: Mol2 Molecule Summary
 - SDF: SD Molecule Summary
 - Smiles: Canvas 2D-JNI
 - CML: CML String
 - CTab: CTab String
 - ChemDraw XML: CDXML String
 - Inchi: Default
 - Molfile: Molfile String
 - Rxn: Rxn String
 - Smarts: Default
 - Sybyl Line Notation: Default
- Other

Grouped structures in a cell

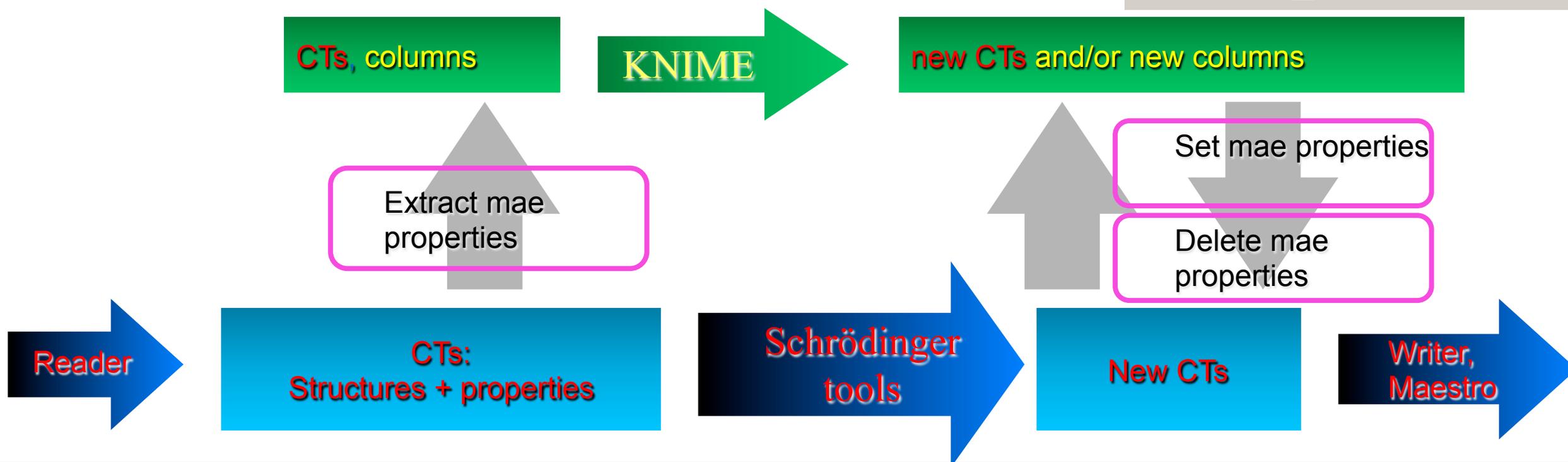
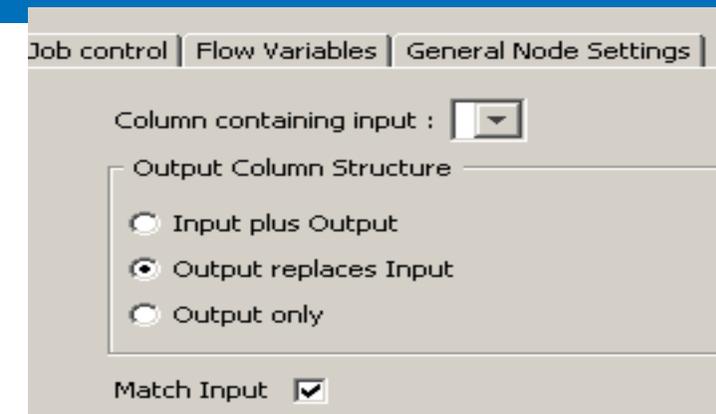
- #CTs: number of structures
- Set of conformations, Glide poses, Ligprep forms...
- Group and ungroup nodes, match option
- Also grouped SD, mol2

Row ID	CT	S s_m_title	i activ
Row1	Molecule: 1AC8 #atoms:...	1AC8	1
Row2	Molecule: 1AET #atoms: 13	1AET	1
Row3	Molecule: 1AC4 #atoms:...	1AC4	1
Row4	?	2AS6	1
Row5	Molecule: 2AS4 #atoms: 14	2AS4	1
Row6	Molecule: 2EUQ #atoms:...	2EUQ	1
Row7	Molecule: 2AS3 #atoms: 13	2AS3	1
Row8	Molecule: 1AEE #atoms: 12	1AEE	1
Row9	#CTs: 2	2EUR	1
Row10	#CTs: 3	1AEU	1
Row11	Molecule: 1AEJ #atoms: 14	1AEJ	1
Row12	#CTs: 3	2EUU	1
Row13	#CTs: 3	1AEQ	1



Output column structure options

- Input plus Output, Output replaces Input, Output only
- Extract MAE properties, Set MAE properties and delete MAE properties nodes



Output column structure options

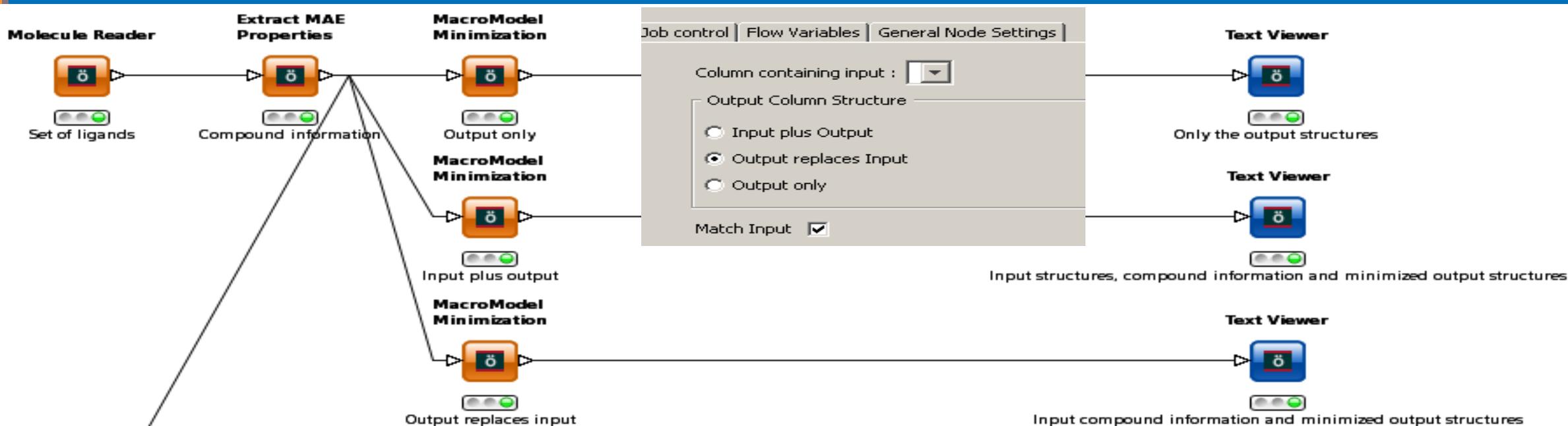
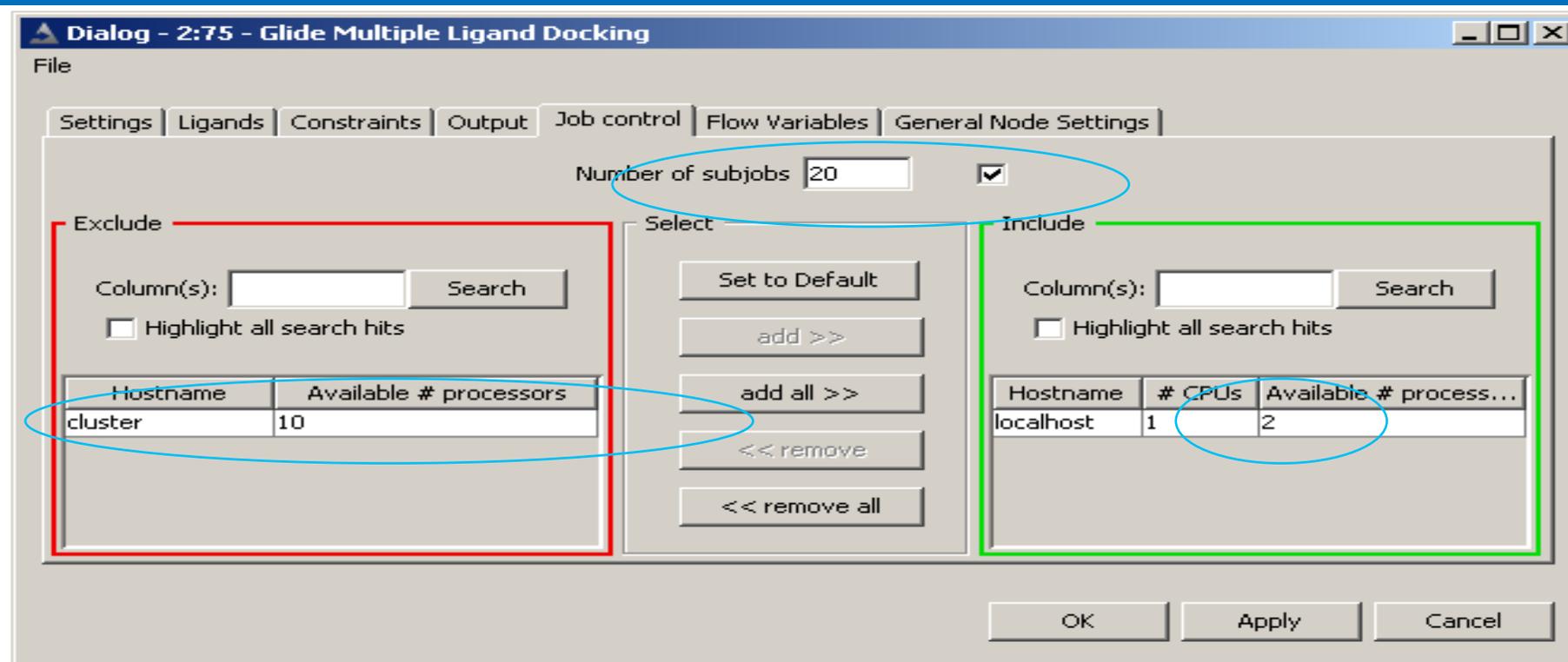


Table View - 2:158 - Text Viewer (Input structures, compound information and minimized output structures)

Row ID	CT_input	s_knime_origin_directory	s_s_knim...	s_s_knim...	s_s_m_entry_...	s_s_m_title	CT
Row0	Molecule: 35 #atoms: ...	/tmp/knime_workflow_example_data/ligan...	50lig.mae	workstatio...	dl-400mw-cul...	35	Molecule: 35 #atoms: ...
Row1	Molecule: 141500 #at...	/tmp/knime_workflow_example_data/ligan...	50lig.mae	workstatio...	dl-400mw-cul...	141500	Molecule: 141500 #at...
Row2	Molecule: 151943 #at...	/tmp/knime_workflow_example_data/ligan...	50lig.mae	workstatio...	dl-400mw-cul...	151943	Molecule: 151943 #at...
Row3	Molecule: 165006 #at...	/tmp/knime_workflow_example_data/ligan...	50lig.mae	workstatio...	dl-400mw-cul...	165006	Molecule: 165006 #at...
Row4	Molecule: 177616 #at...	/tmp/knime_workflow_example_data/ligan...	50lig.mae	workstatio...	dl-400mw-cul...	177616	Molecule: 177616 #at...
Row5	Molecule: 184284 #at...	/tmp/knime_workflow_example_data/ligan...	50lig.mae	workstatio...	dl-400mw-cul...	184284	Molecule: 184284 #at...
Row6	Molecule: 193459 #at...	/tmp/knime_workflow_example_data/ligan...	50lig.mae	workstatio...	dl-400mw-cul...	193459	Molecule: 193459 #at...
Row7	Molecule: 290782 #at...	/tmp/knime_workflow_example_data/ligan...	50lig.mae	workstatio...	dl-400mw-cul...	290782	Molecule: 290782 #at...
Row8	Molecule: 334669 #at...	/tmp/knime_workflow_example_data/ligan...	50lig.mae	workstatio...	dl-400mw-cul...	334669	Molecule: 334669 #at...
Row9	Molecule: 399636 #at...	/tmp/knime_workflow_example_data/ligan...	50lig.mae	workstatio...	dl-400mw-cul...	399636	Molecule: 399636 #at...

Jobcontrol





- Schrödinger preferences
- Start-up script options
- Access to flow variables



- Schrödinger node repository
- Configuration panel visual coherence
- Nodes of general use:
 - Readers and converters
 - Run Maestro and Run Maestro command
 - Structure manipulation
 - Data manipulation and viewers
 - Scripting
- KNIME workflow webpage

Access to Schrödinger tools via KNIME

- Run on Linux, Mac and Windows 32 and 64 bit
- Add our extensions to an existing KNIME installation using the update site
- 150+ nodes covering the whole Schrödinger Suite

Molecular Mechanics

- MacroModel Single Point Energy
- MacroModel Minimization
- MacroModel Coordinate Scan
- ConfGen Standard
- ConfGen
- Conformational Search
- Conformational Search and Cluster
- Premin
- Impref
- Uffmin

Quantum Mechanics

- Jaguar Single Point Energy
- Jaguar Minimization
- NMR Shielding Constants
- Jaguar Charges

Cheminformatics

Fingerprint Based Tools

- Fingerprint Generation
- Generate Pairwise Matrix
- Generate Pairwise Matrix (2 Inputs)
- Similarity Matrix (from Molecules)
- Dissimilarity Selection (from Matrix)
- Build Report for Clustering (from Matrix)
- Hierarchical Clustering (from Matrix)

Filters and Mining Tools

- Maximum Common Substructure Search
- Substructure Search
- REOS Filter
- Structure Filter

Utilities and Converters

- Principal Components
- Multi-dimensional Scaling
- Combine Fingerprints
- Concatenate Bitvectors
- Convert Fingerprint to Bitvector
- Convert Fingerprint to Table
- Convert Matrix to Table
- Convert Table to FingerPrint
- Convert Table to Matrix
- Convert Bitvector to FingerPrint

Modeling

- Bayes Classification Model Building

Pharmacophore Modeling

- Phase Shape
- Phase DB Query
- Phase File Query
- Phase DB Creation
- Phase Hypothesis Identification

Docking and Scoring

- Glide Grid Generation
- Glide Ligand Docking
- Glide Multiple Ligand Docking
- XP Visualizer

Post-processing

- Prime MM-GBSA
- Embrace Minimization
- Strain Rescore
- Pose Entropy
- Pose Filter
- Glide Ensemble Merge
- Glide Merge

Protein Structure Prediction

- BLAST
- Prime Build Homology Model
- Prime Side Chain Sampling
- Prime Minimization

Schrödinger nodes

Workflows

- Protein Preparation
- Protein Preparation Wizard
- Protein Assignment
 - Induced-fit docking
- IFD and individual steps

Ligand Preparation

- LigPrep
- Ligprep individual tools (Ionizer, Desalter, Neutralizer...)
- Epik

Property Generation

- QikProp
- Molecular Descriptors
- Calculate properties

Filtering

- Ligfilter
- Ligparse
- Property Filter (Propfilter)

Scripting

- **Run Maestro Command**
- **Chemistry External Tool** 0:1, 1:0, 1:1, 1:2, 2:1 and 2:2 nodes
- **Python Script** 0:1, 1:0, 1:1, 1:2, 2:1 and 2:2 nodes

Desmond

- System builder
- Molecular Dynamics
- Trajectory extract frames and manipulation
- Trajectory reader, CMS reader

Reporting

- Run Maestro
- Run Canvas
- View CSV (open xls/ooffice)
- Text Viewer

Tools

Combinatorial Libraries

- CombiGlide Library Enumeration
- CombiGlide Reagent Preparation

Fragments

- Fragment Joiner
- Fragments from Molecules

Data Manipulation

Compare Ligands

Lookup and Add Columns

Group MAE

Ungroup MAE

Structure Manipulation

- Add Hydrogens
- **Delete Atoms**
- **Split by Structure**
- **MAE Parser**
- Extract MAE Properties
- Delete MAE Properties
- Set MAE Properties
- Set Molecule Title
- Set MAE Index

Utilities

- Get PDB
- Align Binding Sites
- Protein Structure Alignment
- Prime Fix
- **RMSD**
- Assign Bond Orders
- Unique Title Check
- PDB Name
- SD Format Checker
- Generate Smarts
- Unique Smiles
- Entropy Calculation
- RRHO Entropy
- Boltzmann Population
- Volume Overlap Matrix

Readers/Writers

- CSV Reader
- Molecule Reader
- SD, PDB, Mol2 Reader nodes
- Sequence Reader
- Alignment Reader
- Fingerprint Reader
- Hypothesis Reader
- Glide Grid Reader
- Glide Multiple Grid Reader
- Variable Based Glide Grid Reader
- Molecule Writer
- Sequence Writer
- Alignment Writer
- Hypothesis Writer
- Fingerprint Writer

Converters

- Molecule-to-MAE
- MAE-to-Pdb, to-SD, to-Smiles and to-Mol2
- SD-to-Smiles
- PoseViewer-to-Complexes
- Complexes-to-PoseViewers
- String-to-Type
- Hartree-to-kcal/mol Converter
- kJ-to-kcal Converter

Visual Coherence – Maestro vs. KNIME

Read in
Ligands

Smiles Reader



Read 2D Ligands

LigPrep

Use structures from: **File**

File name: **Browse...**

Filter criteria file: **Create...** **Browse...**

Force field: **OPLS_2005**

Ionization:

Retain original state

Neutralize (best for QikProp)

Generate possible states at target pH: +/-

Using:

Ionizer

Epik

Add metal binding states

Desalt Generate tautomers

Stereoisomers

Computation:

Retain specified chiralities (vary other chiral centers)

Determine chiralities from 3D structure

Generate all combinations

Generate at most: per ligand

Generate low energy ring conformations: per ligand

Output format: Maestro SDF

Start... **Close** **Help**

Read in
Grid

Dialog - 2:3 - LigPrep (2D -> 3D)

File

Ligprep Job control Flow Variables General Node Settings

Column containing input: **SMI Smiles**

Output Column Structure

Input plus Output

Output replaces Input

Output only

Match Input

Force field: **OPLS_2005**

Ionization:

Retain original state

Neutralize (best for QikProp)

Generate possible states at target pH: +/-

Using:

Ionizer

Epik

Add metal binding states

Desalt Generate tautomers

Stereoisomers

Computation:

Retain specified chiralities (vary other chiral centers)

Determine chiralities from 3D structure

Generate all combinations

Generate at most: per ligand

Generate low energy ring conformations: per ligand

Output Type: **Maestro**

OK **Apply** **Cancel**

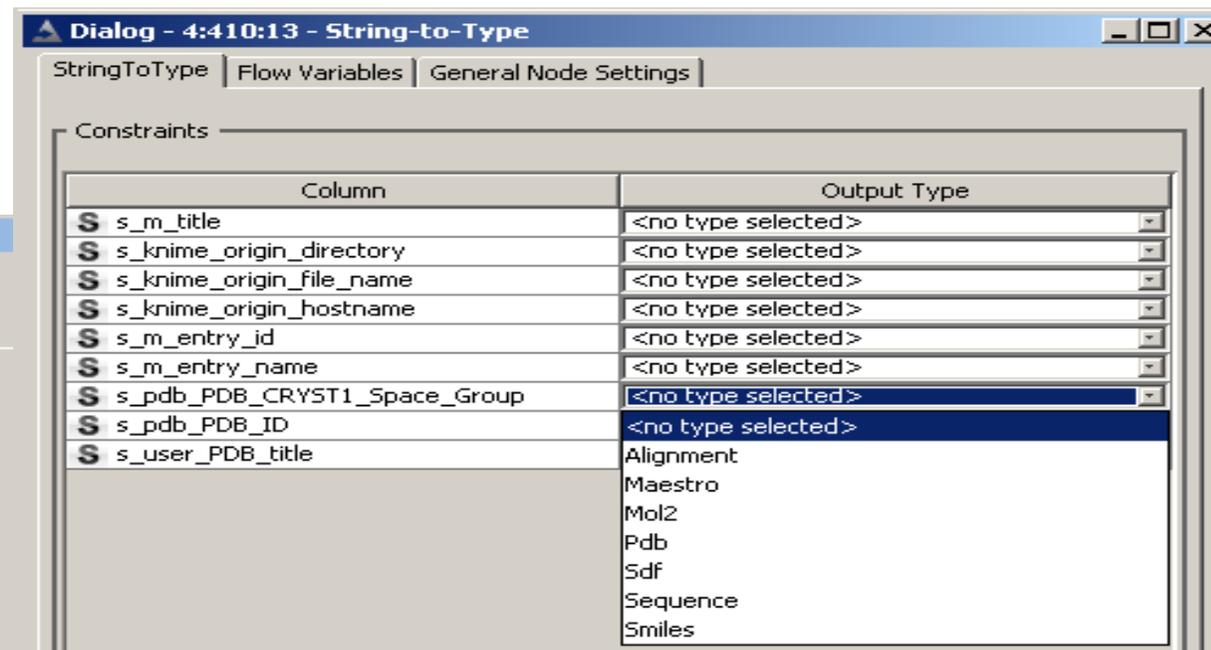
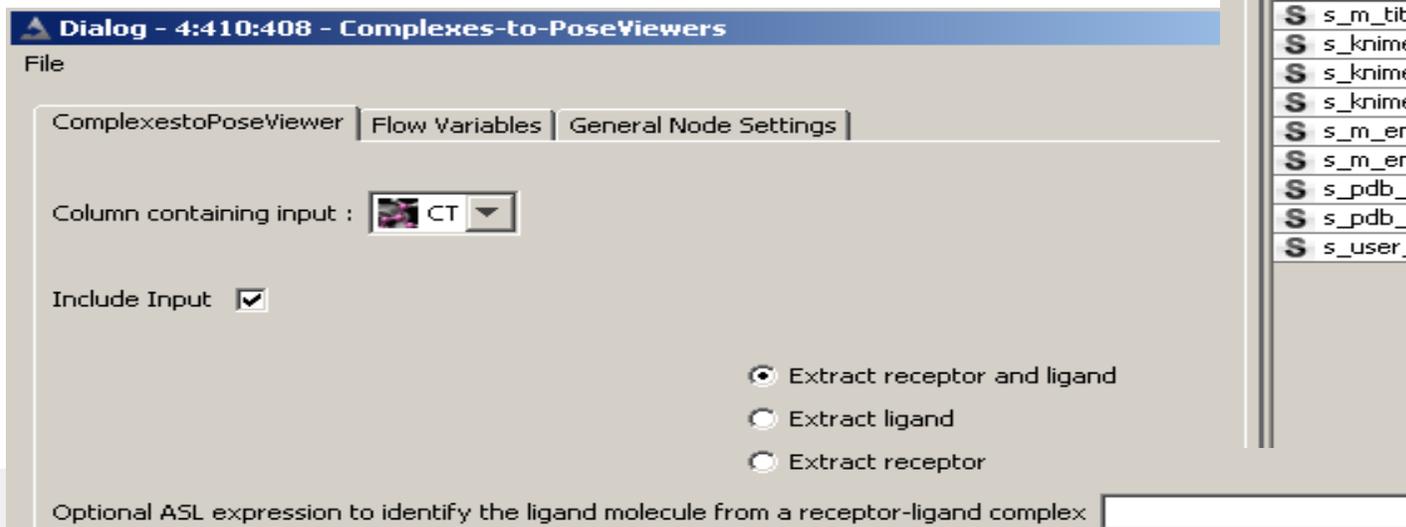
Maestro

05

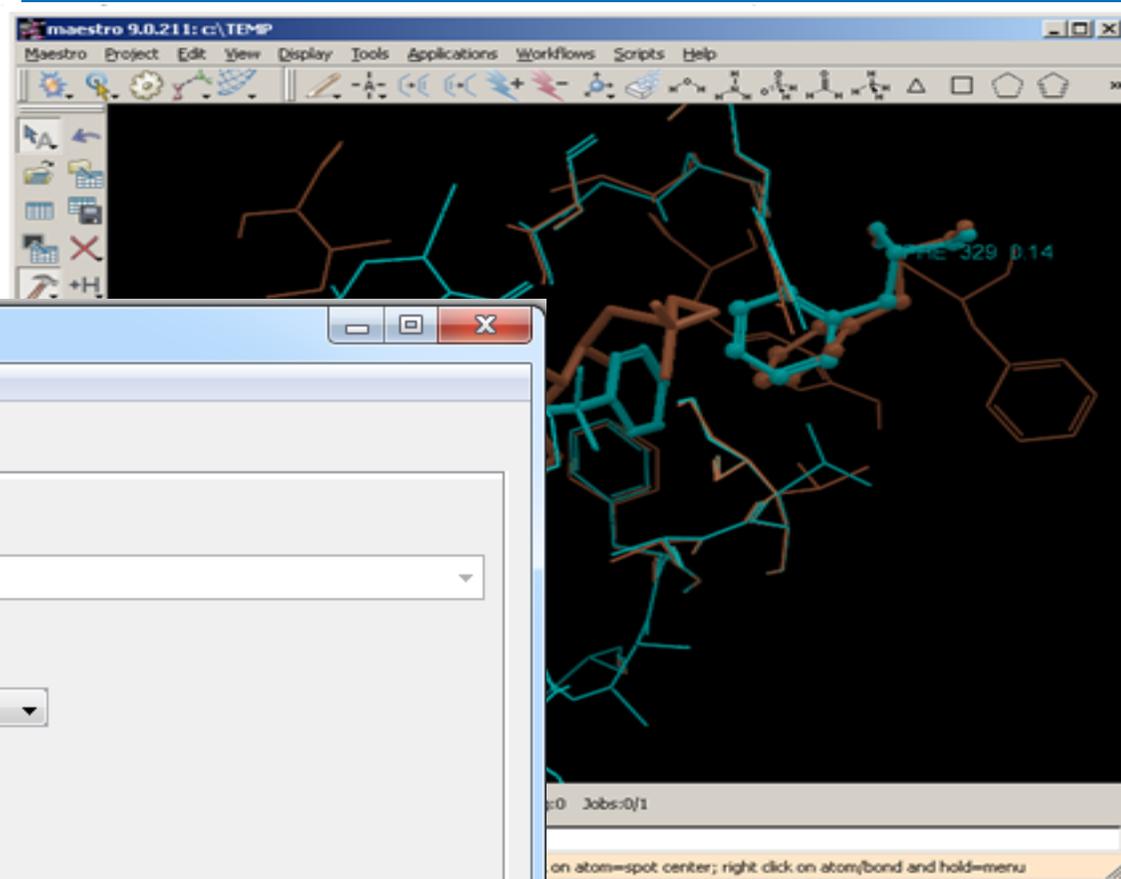
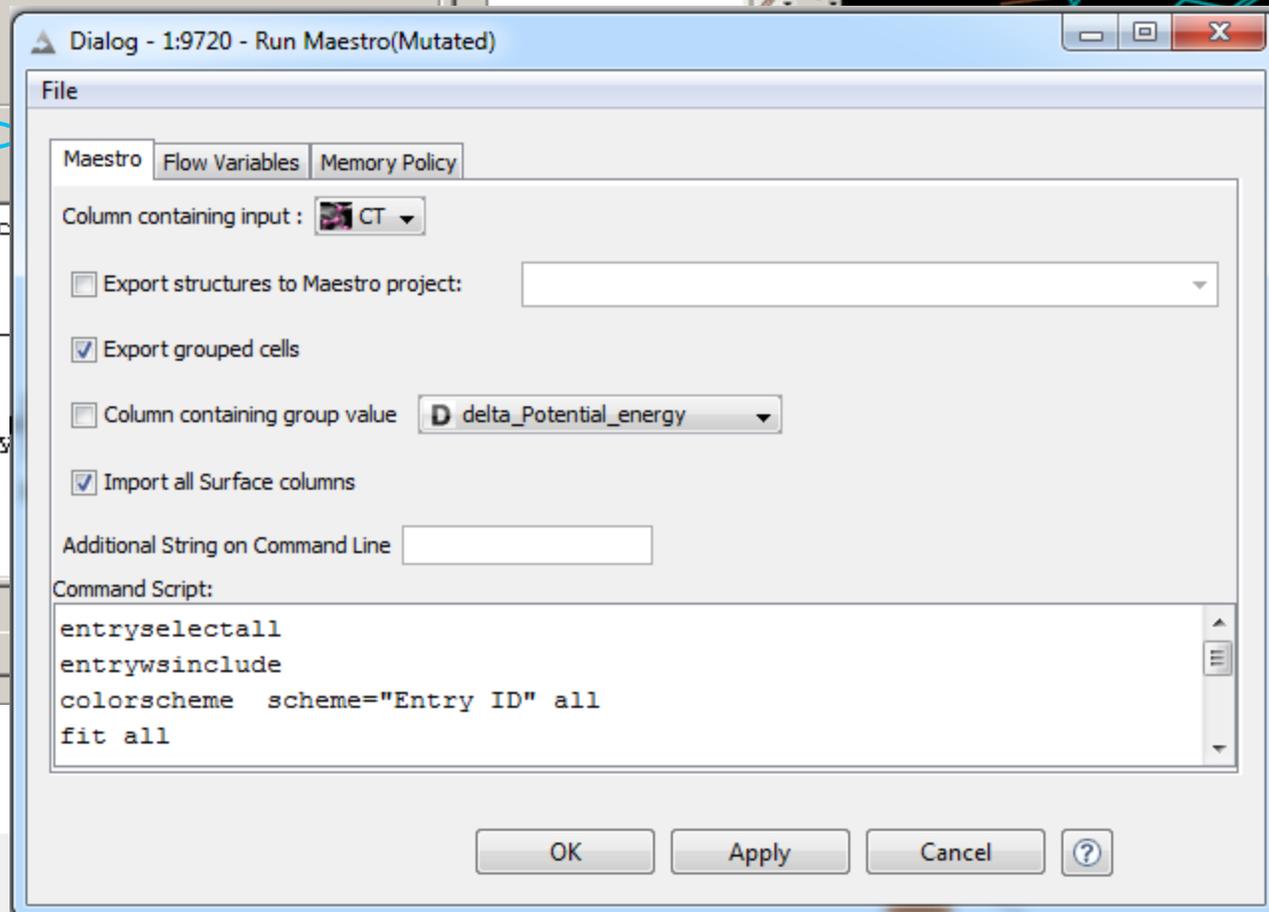
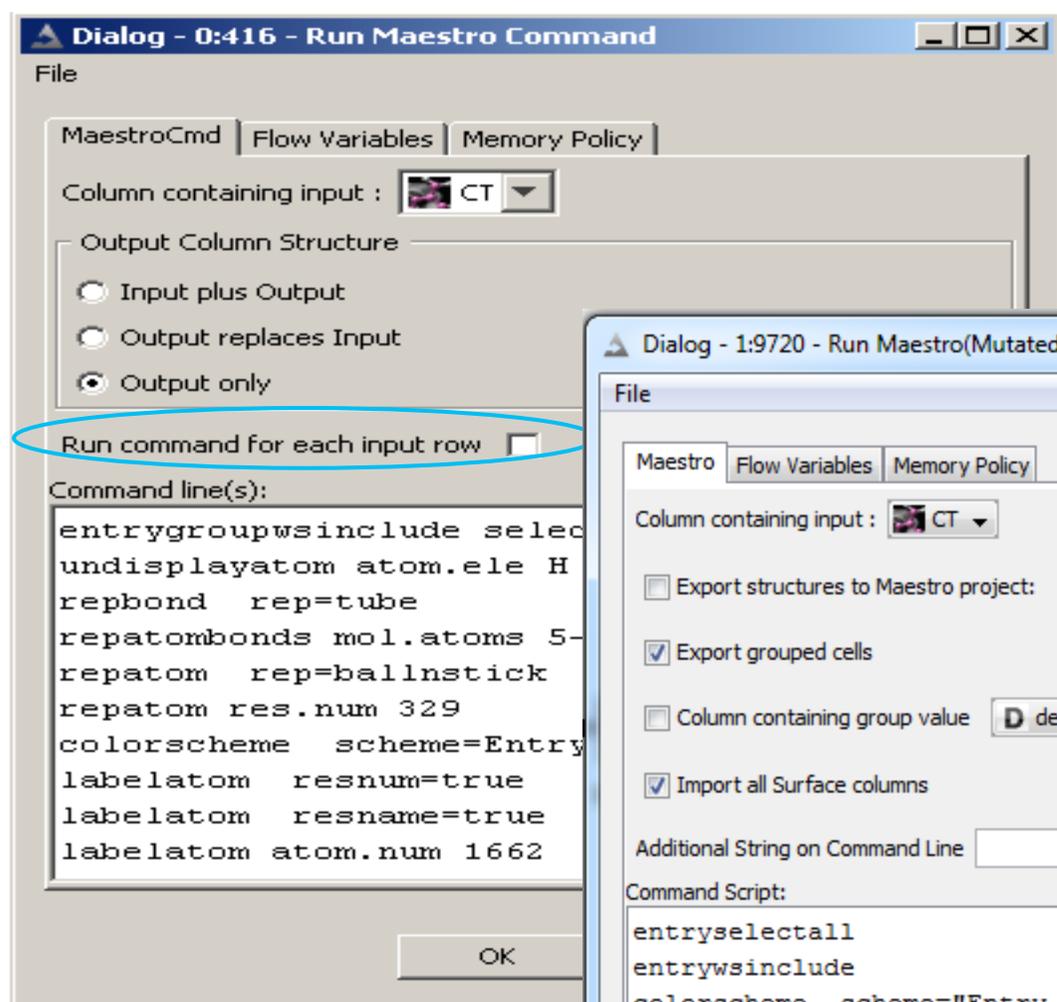
GER.

Nodes of general use - Readers and converters

- Molecule reader, SD reader... Glide grid reader...
- Converters (Maestro, mae.gz, SD, sd.gz, mol2, PDB, smiles) including Molecule to MAE, string to type. Canvas converters (Matrix, Fingerprint, Bitvector from and to table). SD format checker
- Pose viewer to complexes and Complexes to PoseViewer



Run maestro command and Run Maestro



Nodes of general use - Structure manipulation

- Set MAE properties

Short Column Names in Output:

Rescan input: Rescan Input Automatically:

Exclude

Column(s): Search

Highlight all search hits

- S s_knime_origin_directory
- S s_knime_origin_file_name
- S s_m_entry_name
- I i_mmod_Conformation-OPLS-2005
- I b_mmod_Minimization_Converged-OPLS-2005
- D r_mmod_Potential_Energy-OPLS-2005
- D r_mmod_Relative_Potential_Energy-OPLS-2005
- I i_mmod_Times_Found-OPLS-2005

Select

Families: MacroModel('mmod')

add >>

add all >>

<< remove

<< remove all

New Property:

User-defined property type

String Integer Double

add user-defined >>

Include

Column(s): Search

Highlight all search hits

- S s_m_title
- S s_knime_origin_hostname
- D r_mmod_RMS_Derivative-OPLS-2005
- I # atoms
- I # bonds

OK Apply Cancel

Dialog - 6:161 - Set MAE Properties (for the table column)

File

MAESetProperties | Flow Variables | General Node Settings

Column containing input: CT

Output Column Structure

- Input plus Output
- Output replaces Input
- Output only

Set all properties to column names

Set selected properties to column names

Clear all properties

Properties

Column Name	Column Type	Prefix/source	Property	Actual Property
s_knime_origin_...	String	knime	origin_directory	s_knime_origin_directory
s_knime_origin_...	String	knime	origin_file_name	s_knime_origin_file_name
s_knime_origin_...	String	knime	origin_hostname	s_knime_origin_hostname
s_m_entry_name	String	m		
s_m_title	String	m		

OK

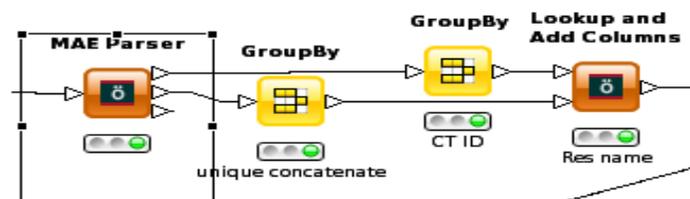
Apply

Cancel

- Extract MAE properties

Nodes of general use - Structure manipulation

- Extract and Set MAE properties
- Group and Ungroup, Set MAE index
- MAE parser
- Split by structure, Delete atoms
- Compare ligands
- Unique smiles, Unique title check, Ligfilter, Align binding sites, RMSD, Volume overlap matrix...



Atom properties - 2:1451:1100 - MAE Parser

Row ID	ct-id	atom-id	i_m_m...	D_r_m_x...	D_r_m_y...	D_r_m_z...	i_m_re...	S_s_m_in...	S_s...
Row 1	1	1	2	41.858	7.688	24.757	100		X
Row 2	1	2	15	41.794	8.906	24.854	100		X
Row 3	1	3	3	41.806	6.775	25.963	100		X
Row 4	1	4	25	42.111	7.042	23.642	101		X
Row 5	1	5	3	42.191	7.68	22.362	101		X
Row 6	1	6	2	41.047	7.296	21.464	101		X
Row 7	1	7	15	40.64	6.12	21.387	101		X
Row 8	1	8	3	43.446	7.282	21.676	101		X
Row 9	1	9	2	44.659	7.788	22.399	101		X
Row 10	1	10	2	45.301	6.953	23.288	101		X

Column containing input :

Output Column Structure

Input plus Output

Output replaces Input

Output only

ASL Expression

Nodes of general use - Data manipulation and viewers

- Look up and add columns
- Run Spreadsheet viewer(OpenOffice/Excel)
- Table viewer

Table View - 5:43 - Text Viewer (Check the Force field parameter quality) (3 x 4)

Row ID	CT	Log Log_input
Row1	#CTs: 4	STARTUP COMMAND: time /usr/local/schro-latest/macromodel-v97211/bin/Linux-x86_64/bmin MMSHARE_EXEC: /usr/local/schro-latest/mmshare-v18212/bin/Linux-x86_64 JobID: workstation2-3-4ae18bb2 BatchMin V9.7 Build 97211 Starting Time 23-Oct-2009 12:55:59 MacroModel. Copyright (c) 2009 Schrodinger, LLC. All rights reserved. ConfGen V2.1 Build 21211 Input filename: mmconfgen_job_512298853_in_1.mae Output filename: mmconfgen_job_512298853_1-out.mae Turning on debug switch 3 Atom-type file: /usr/local/schro-latest/mmshare-v18212/bin/Linux-x86_64/../../data/atom.typ Force field: /usr/local/schro-latest/macromodel-v97211/bin/Linux-x86_64/../../data/OPLS_2005.fld Read 29 atoms. Structure name, if any, appears on next line: mol_0004 CGEN: Using ring conformation library. CGEN: Number of ring conformations generated: 16
Row2		
Row3		

Row: Row1
Column: Log_input
Type: LogFileCell

Dialog - 4:30 - Lookup and Add Columns (Groups tha...
File

LookupAndAdd | Flow Variables | General Node Settings

Key column : S MCS_ID
Lookup column : S s_canvas_MCS_ID
Include column : CT

Include One Column
Include All Columns

Add String to column names in Input 2 (if duplicate) _found
Use Hash (Keep all necessary data in memory)

OK Apply Cancel

Preferences

type filter text

Schrödinger

Schrödinger global preferences

Directory for temporary files c:\TEMP Browse...
Default Host localhost (2)
 Delete temporary files after a node successfully executes
Number of log lines shown when a node fails 50
Open Office Spreadsheet Command Line oocalc

Recheck license

KNIME Workflows Available for Download

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KNIME Workflows

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KNIME Workflows

Select Workflows

Cheminformatics

Docking / Docking Post-processing

General Tools

Labs

Library Design

Molecular Dynamics

Pharmacophore Modeling

Protein Modeling

Quantum Mechanics

Real World Examples

Workbench

Important Notes

KNIME Workflows | or "[Click here](#)" for KNIME Workflows for

KNIME Workflows for **Schrödinger Suite 2013-3** can be downloaded from

If you require the workflows for Schrödinger Suite 2013-2, please [click here](#)

Below are many useful workflows for performing automation, customization, augmentation to the Schrödinger Suite. The workflows additionally provide scientists to create custom workflows. Check back regularly, as improved workflows and new workflows are added frequently. Send requests for improved new workflows to help@schrodinger.com.

Select Workflows

Listed below are example KNIME Workflows that utilize many of the Schrödinger (Nodes) as well as many other built-in tools.

- **Cheminformatics**
- **Docking / Docking Post-processing**
- **General Tools**
- **Labs**
- **Library Design**
- **Metanodes**
- **Molecular Dynamics**
- **Molecular Mechanics**
- **Pharmacophore Modeling**
- **Protein Modeling**
- **Quantum Mechanics**

Cheminformatics

- Cluster by Fingerprint:** Cluster structures by fingerprints and inspect the clustering statistics to choose a good number of clusters. Create automatically the optimum number of clusters based on the Kelley penalty. Select diverse representatives per cluster. [1 (2.1), 1-2 (1.2), 1-3 (2.3), 1-4 (2.7)] [Requires: Canvas] 03/17/2012
- Database Analysis:** Assess the coverage of a database from the distribution of the distance to the nearest neighbor of each molecule in the database. List the three most similar compounds for each compound in the database. [1 (3.7), 1-2 (3.7)] [Requires: Canvas] 03/17/2012
- Maximum Common Substructure Search (MCSS):** Create all possible MCS groups and list the groups identified. Inspect the compounds in the first group and list the compounds that aren't included in this group. List the MCS groups that contain a compound of interest. Create all the groups with the option limiting each compound to at most one MCS group and present the structures in these groups in a matrix. [1 (2.1), 1-2 (2.1), 1-3 (2.1), 1-4 (2.1)] [Requires: Canvas] 04/01/2011
- Select Diverse Molecules:** Pick diverse molecules from a library and inspect the structures. [1 (1.1)] [Requires: Canvas] 11/02/2009
- Similarity Search:** Find the most similar compounds to a sketched molecule in a database. Screen the same database against several query structures. [1 (2.1), 1-2 (3.7)] [Requires: Canvas] 04/29/2013
- Substructure Search:** Search a set of structures against a sketched query molecule or SMARTS patterns. Report the compounds that don't pass all the REOS filters. [1 (2.1), 1-2 (5.1)] [Requires: Canvas] 04/29/2013

Docking / Docking Post-processing

- SiteMap:** A set of PDB structures is prepared, possible binding sites identified with SiteMap and visualized in Maestro. A set of ligand binding site regions are characterized. [(6.0)] [Requires: SiteMap] 04/29/2013

<http://www.schrodinger.com/knimeworkflows>

Other KNIME Workflows

Cheminformatics

- Cluster by Fingerprint
- Database Analysis
- Maximum Common Substructure Search (MCS)
- Select Diverse Molecules
- Similarity Search
- Substructure Search

Docking and Post-Processing

- Docking and Scoring
- Ensemble Docking
- Loop Over Docking Parameters
- Protein Preparation and Glide Grid Generation
- Validate Docking Parameters
- Virtual Screening
- SiteMap

Pharmacophore Modeling

- Phase Hypothesis Identification
- Phase Screening
- Shape Screening

Molecular Dynamics:

- Desmond Simulation

Molecular Mechanics

- Compare Conformational Search Methods
- Conformational Search and Post-Processing

Quantum mechanics

- Conformational Search and QM Refinement
- ESP Charges
- Jaguar pKa
- Quantum Mechanical Properties
- Semi-empirical Optimization

Library Design

- Library Enumeration

Protein Modeling

- Induced Fit Docking Protocol
- Model Building

Workbench

- Group By Use-cases
- Group Looper
- Unpivot

Real World Examples

- Binding Site Shape Clustering
- Sitemap and Glide Grid Generation
- Vendor Database Preparation

Labs

- Glide Grid Writer
- Parameter Flow Variable Use-cases
- Run Maestro 1:1 Use-cases

General tools

- Chemistry External Tool Use-cases
- Ensure Molecule Title Uniqueness
- Output Column Structure Option Philosophy
- Protein Structure Alignment
- Python Script Node Use-cases
- Run Maestro Command Node Use-cases
- Run PyMOL
- Split and Align Multimers
- Webservice
- Workflows in the Current Workspace

<http://www.schrodinger.com/knimeworkflows/>



- Chemistry tool nodes
- Python nodes
- Row iterator loop start
- Look up and add vs. Joiner node
- Miscellaneous nodes: Compare ligands, Set molecule title

KNIME workbench

- GUI
- Nodes



Schrödinger extensions

- Specificities
- Schrödinger nodes



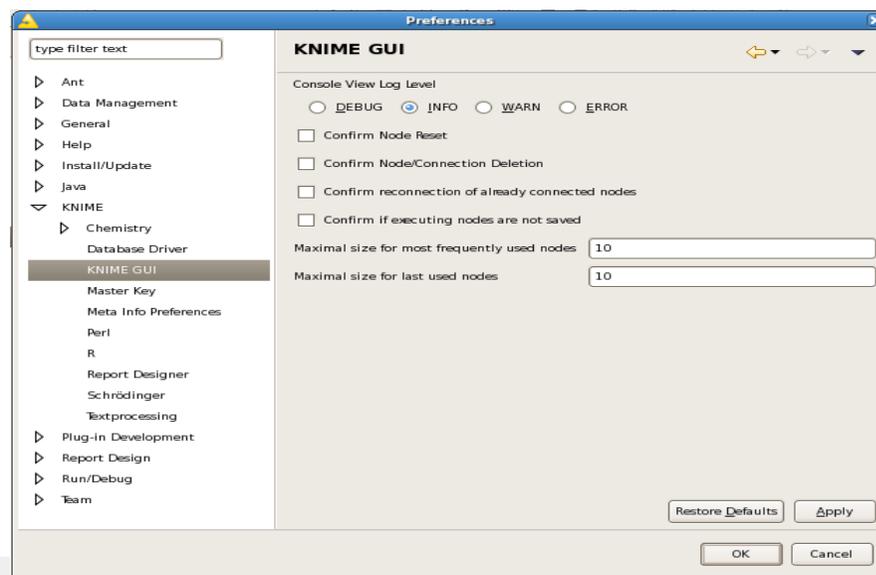
- ◀ Get started
- ▶ Advanced functionalities



- Preferences
- Advanced node functionalities
- Errors, warnings and Console information
- Flow variables and workflow variables
- Metanodes
- Memory limit
- Tips and tricks

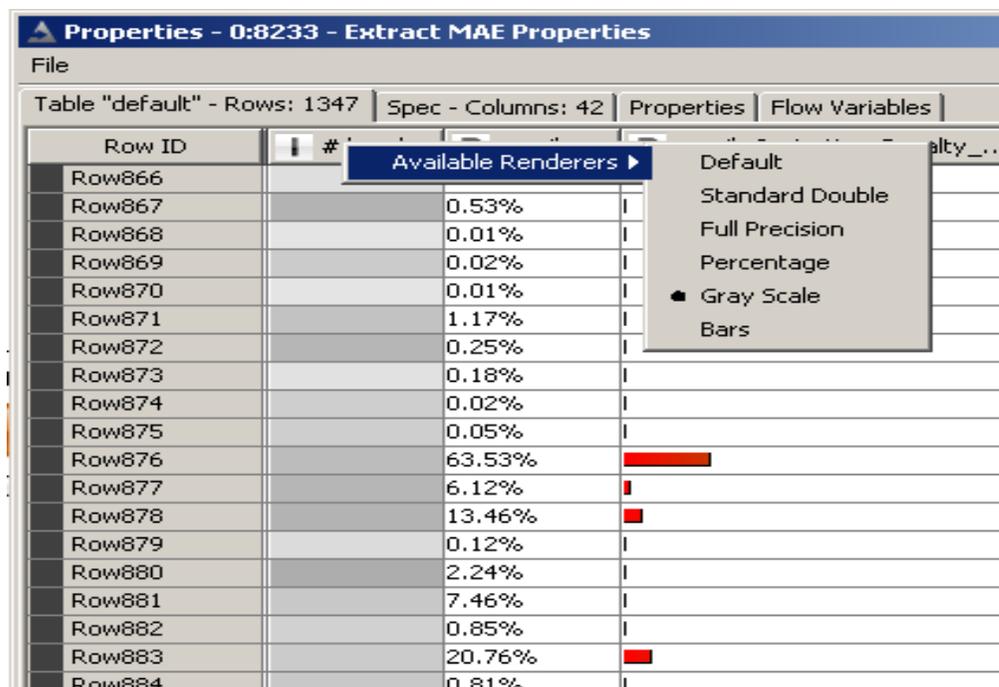
Preferences > KNIME

- Directory for temporary files (See also Schrödinger preferences ►)
- KNIME GUI- disable the node reset, deletion and reconnection confirmation
- KNIME GUI- Console view log level: recommended to change to INFO. Example of information provided by Schrödinger nodes ►



Advanced node functionalities

- Hovering over an input connector tells you what the node takes as input (eg Molecules in Maestro, SMILES or SD format)
- Hovering over an output connector reports the number of rows and columns in the output table
- Comment a workflow: Node pop-up menu > Node name and description
- Data table > change the renderer



The screenshot shows a window titled "Properties - 0:8233 - Extract MAE Properties". The window contains a table with the following data:

Row ID	#	Value	Renderer
Row866			
Row867		0.53%	
Row868		0.01%	
Row869		0.02%	
Row870		0.01%	
Row871		1.17%	
Row872		0.25%	
Row873		0.18%	
Row874		0.02%	
Row875		0.05%	
Row876		63.53%	Red bar
Row877		6.12%	Red bar
Row878		13.46%	Red bar
Row879		0.12%	
Row880		2.24%	
Row881		7.46%	
Row882		0.85%	
Row883		20.76%	Red bar
Row884		0.81%	

A context menu titled "Available Renderers" is open over the table, showing the following options: Default, Standard Double, Full Precision, Percentage, Gray Scale (selected), and Bars.

Errors, warnings and Console information

- Popup-menu > View Std output/error
- Warning sign above the node status when the node completed with potential errors

- Console information:

INFO HierarchicalClusteringNodeModel Preparing input file '/tmp/HierarchicalClustering_in_423741.mat'

INFO HierarchicalClusteringNodeModel Finished preparing file time 0.35 seconds

INFO HierarchicalClusteringNodeModel 10:42:45 11.17.2009:

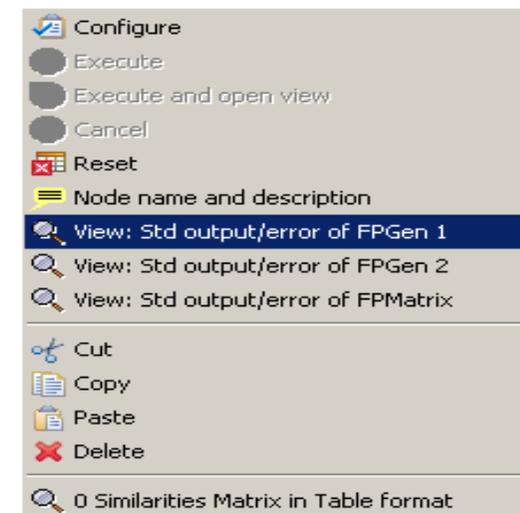
Running cmdline[0]='=/usr/local/schro-latest/utilities/canvasHC -im HierarchicalClustering_in_4116794508031023741.mat -ot HierarchicalClustering_in_4116794508031023741.tree -og HierarchicalClustering_in_4116794508031023741.csv -linkage schrodinger -n 123'

INFO HierarchicalClusteringNodeModel Completed time 1.626 seconds

INFO HierarchicalClusteringNodeModel Preparing output

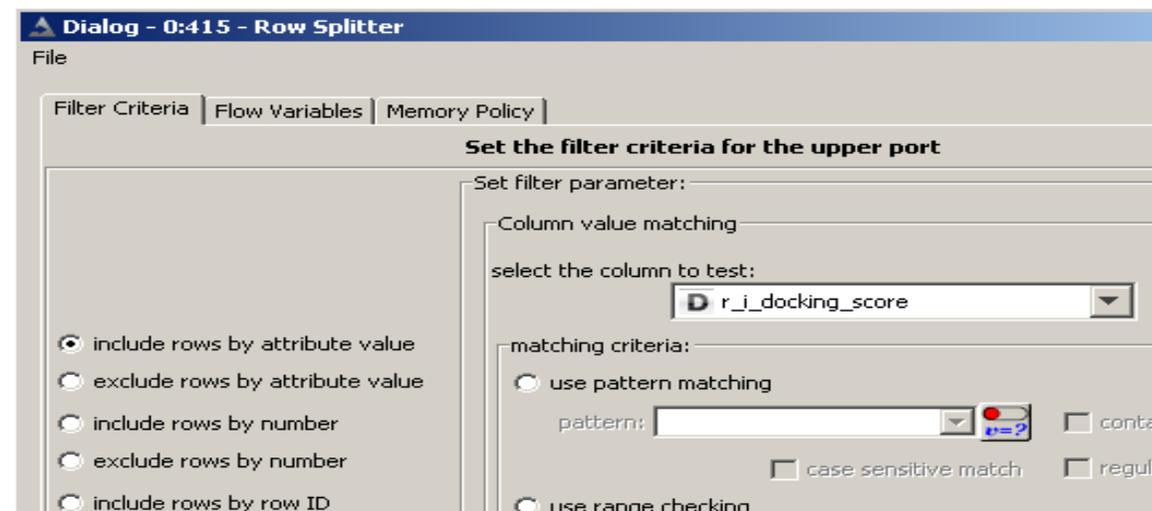
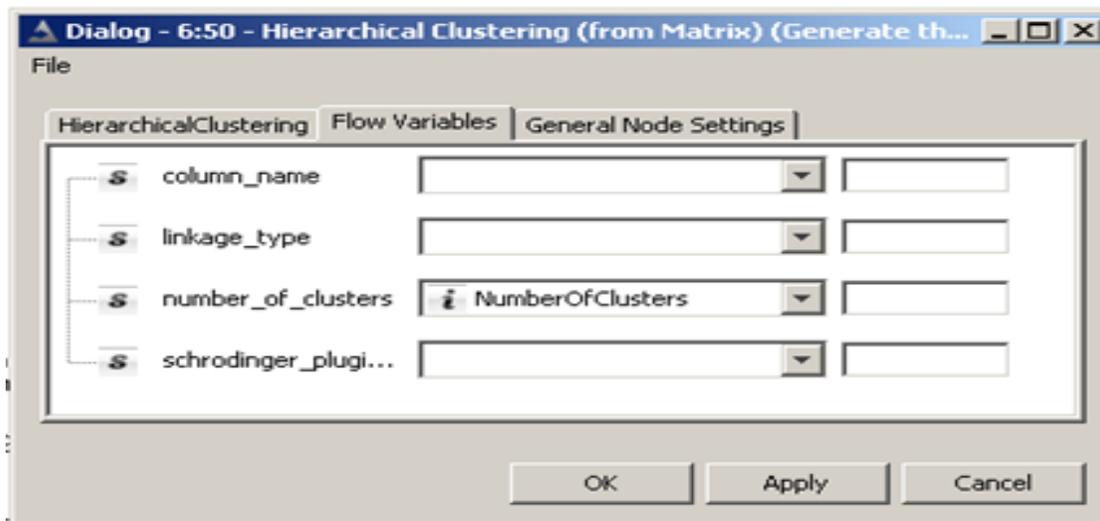
INFO HierarchicalClusteringNodeModel Finished preparing output: time 0.06 seconds

INFO LocalNodeExecutionJob Hierarchical Clustering (from Matrix) 0:2:50 End execute (2 secs)



Flow variables and workflow variables

- The Flow variables are used pass data between nodes on top of the connections.
- In the flow variable tab or the configuration panel for a couple of nodes:



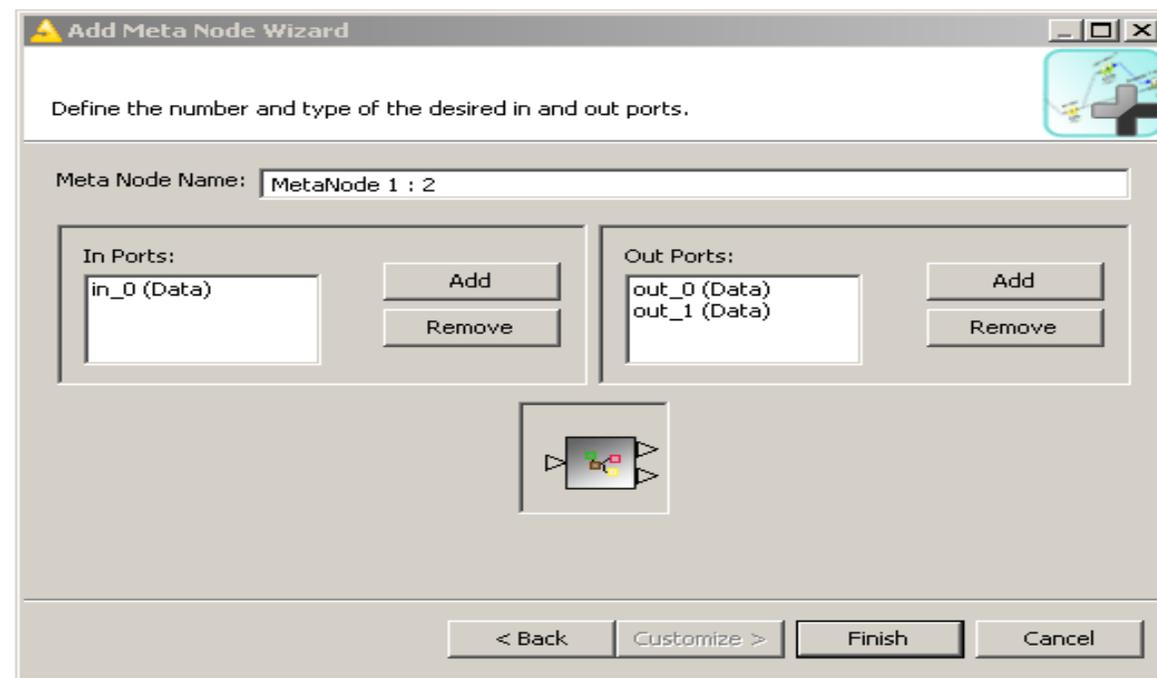
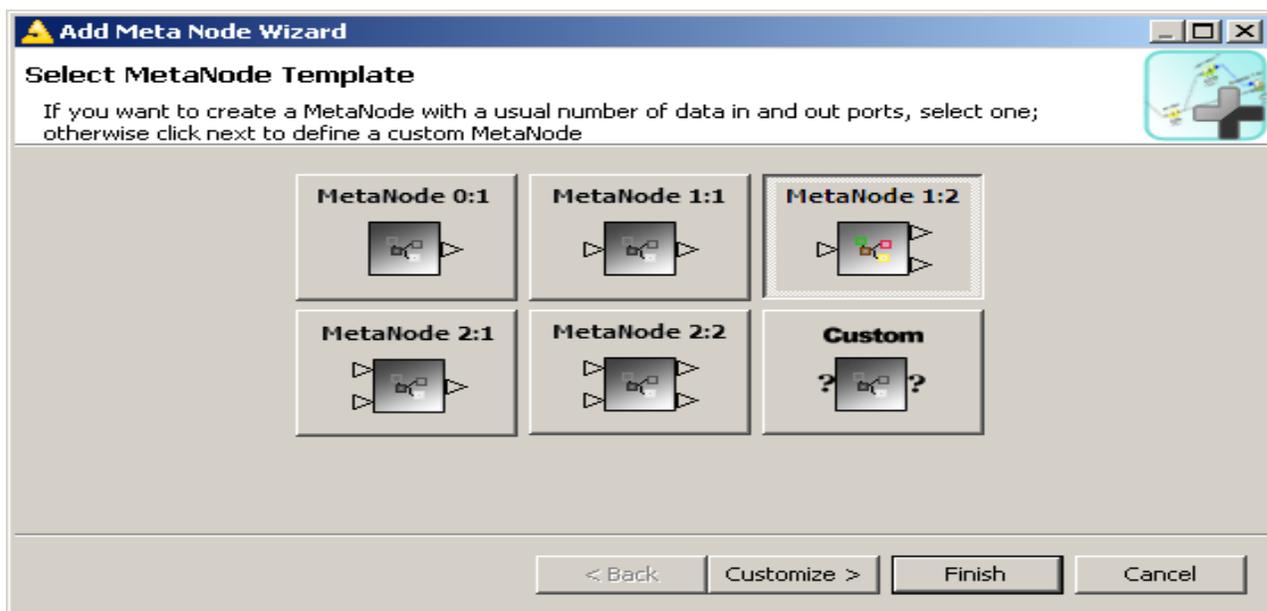
- Global variables can also be set: with the Java snippet node ►

Or in the Workflow project repository select the workflow and Workflow variables in the pop-up menu.

See also Schrödinger specificities ► and nodes to edit variables ►

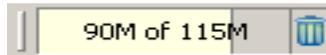
Metanodes

- To hide the complexity and organize a workflow
- Chose the number and type of input/output
- The metanodes open up in new tabs



Memory limit

- Check the memory limit: Help > About Knime > Installation details > Configuration and search for a line starting with "eclipse.vargs=-Xmx" (close to the top).
- Increase the memory allocated to KNIME:
 - `$SCHRODINGER\knime -maxHeap 4096m`
 - `knime -Xmx4096m` (as last option in the command line)
 - in `$SCHRODINGER\knime-v*\bin*\knime.ini`: change `-Xmx1024M` into `2048M` (or higher on 64 bit)
- The error message usually contain "Java heap space" when there is a KNIME is running out of memory.
- Preferences > General > Show heap status and use the garbage collector.
- Knime and Schrödinger tools (eg Canvas) don't compete for memory.



Tips and tricks

- Copy and paste some nodes to a specific place:
Select, copy the nodes (Ctrl+C), right click where you want to paste the nodes and select Paste in the pop-up menu.
Using Ctrl+V instead the nodes will be pasted a little below the original ones.
- The keyboard shortcuts for items on the menus are listed as usual with the menu item. In File > Preferences > General > Keys you can view all the key bindings to commands, modify the bindings, and create your own shortcuts.
- All the branches can be run at the same time using the GUI toolbar Execute all executable nodes button. See also Cancel all running nodes.

Known issues

- If you can't save the workflow with a Java heap space error try to disconnect the last node or run the garbage collector.



- Report designer
- Global variables
- Batch execution
- Tips and tricks



- KNIME.com Labs nodes
- Scripting and run a third party tool
- Java snippet use-cases
- Manipulate the table row IDs using the RowID node
- Aggregation using the GroupBy node
- Miscellaneous nodes: Interactive table, Math formula, CDK Sketcher
- Plotting facilities
- Looping functionalities- Basics
- Model building nodes

KNIME.com Labs nodes

- Pipeline Pilot Connector (other way around?)
- Web Service client, etc

Specific update site: <http://labs.knime.org/>

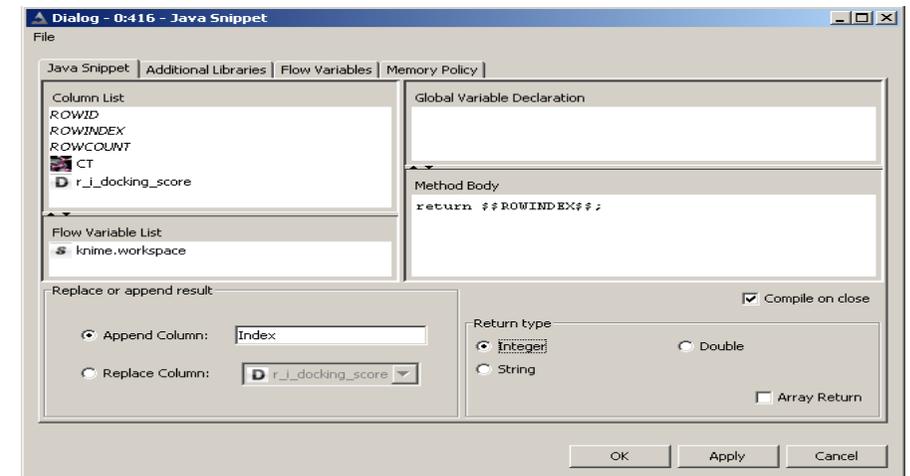
Scripting and run a third party tool

- Java snippet [▶](#)
- Jython and Schrödinger Python nodes [▶](#)
- Perl scripting
- External tool and Schrödinger Chemistry external tool nodes [▶](#)
- Run Maestro commands [▶](#)

Java snippet use-cases

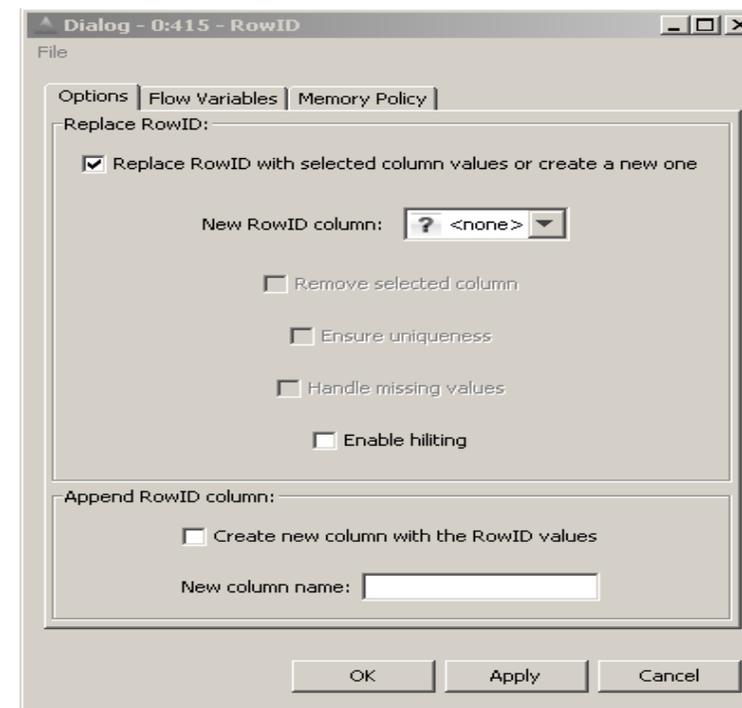
- Duplicate numeric or string columns
- Create a new column from scratch (eg a tag)
- Combine columns (and flow variables) but use the Combiner node for simple tasks
 - eg return "prefix-"+"\$\$FlowVar\$\$+"_ref_"+"\$Col1\$;
- Add a row index (see also Set MAE index)

See the corresponding workflow example.



Manipulate the table row IDs using the RowID node

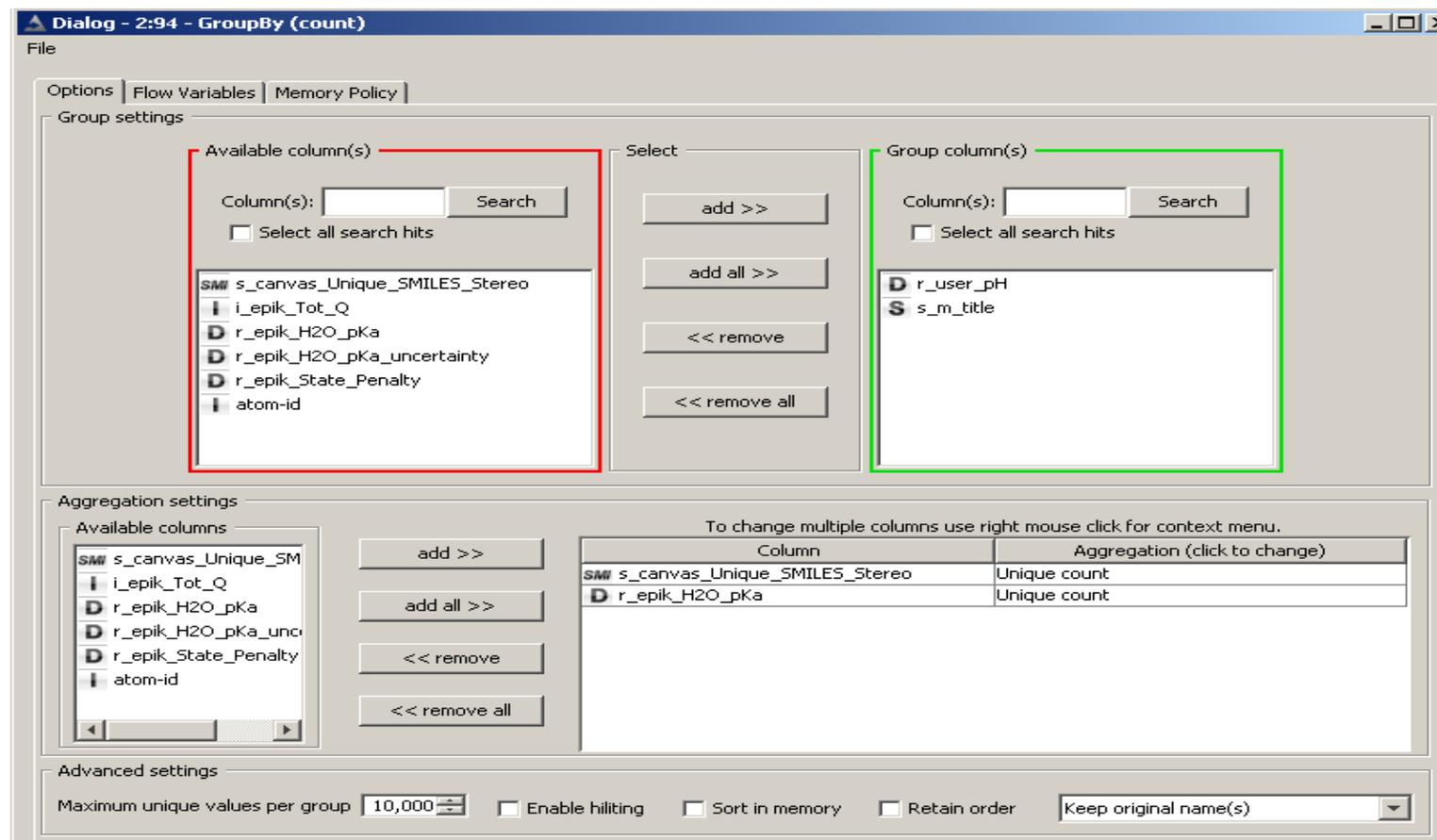
- Use data table column values as row IDs and store Row IDs in a column.
Use-cases:
 - before transposing a data table
 - Set the labels to be used by the Plotter node
- Ensure row ID uniqueness
 - eg for Canvas tools before creating a matrix)



Aggregation using the GroupBy node

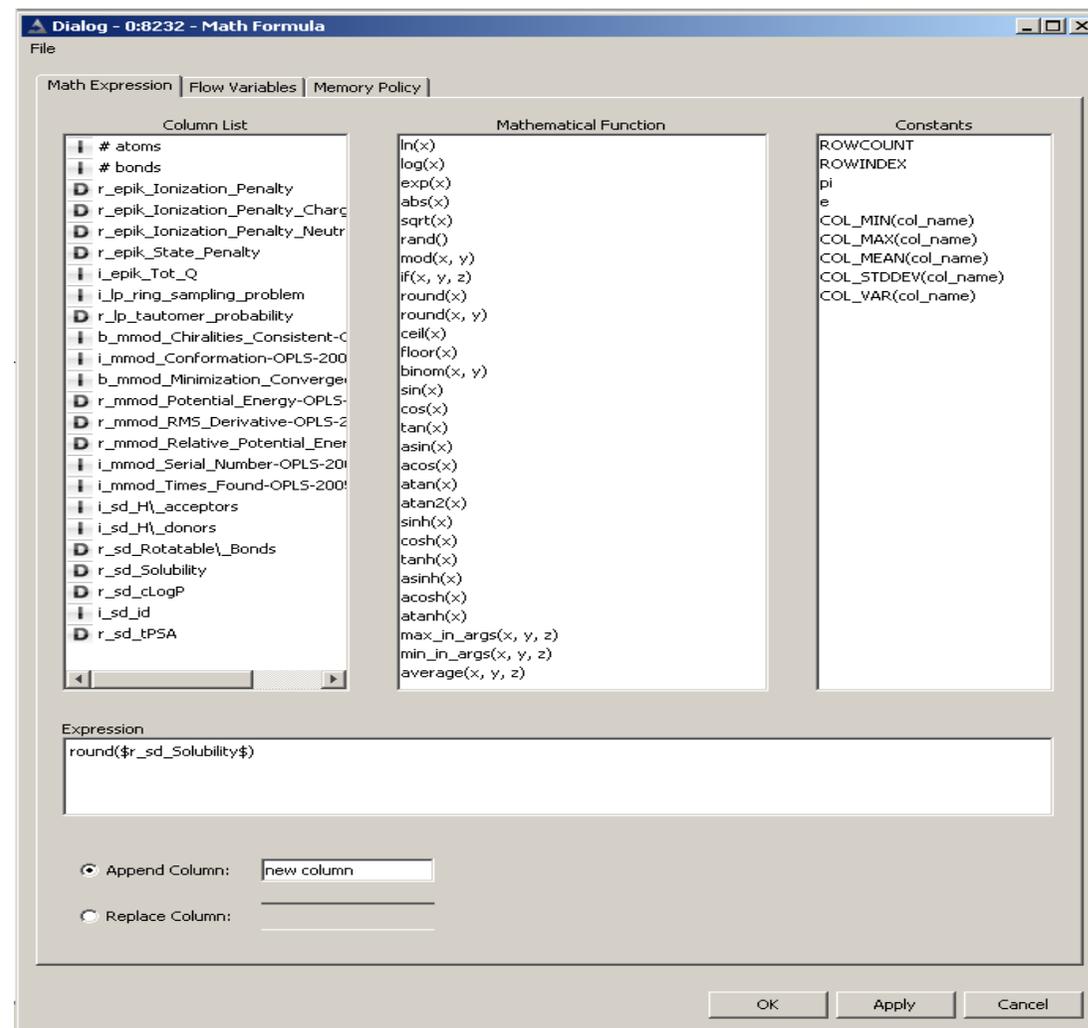
Some of the aggregation methods:

- first, last
- max, min
- Mean
- Sum
- Concatenate
- (unique) count
- List
- Set



Miscellaneous nodes

- Interactive table: Find & Find Next equivalent to the Schrödinger Text viewer node that have more functionalities
- Math formula
- CDK Structure sketcher or Marvin sketch (free of charge from Infocom)



Plotting facilities



- Data Views: Plotter, Histogram...
- Mining > Scoring: Enrichment plotter, ROC curve
- Advanced capabilities available in KNIME Report designer



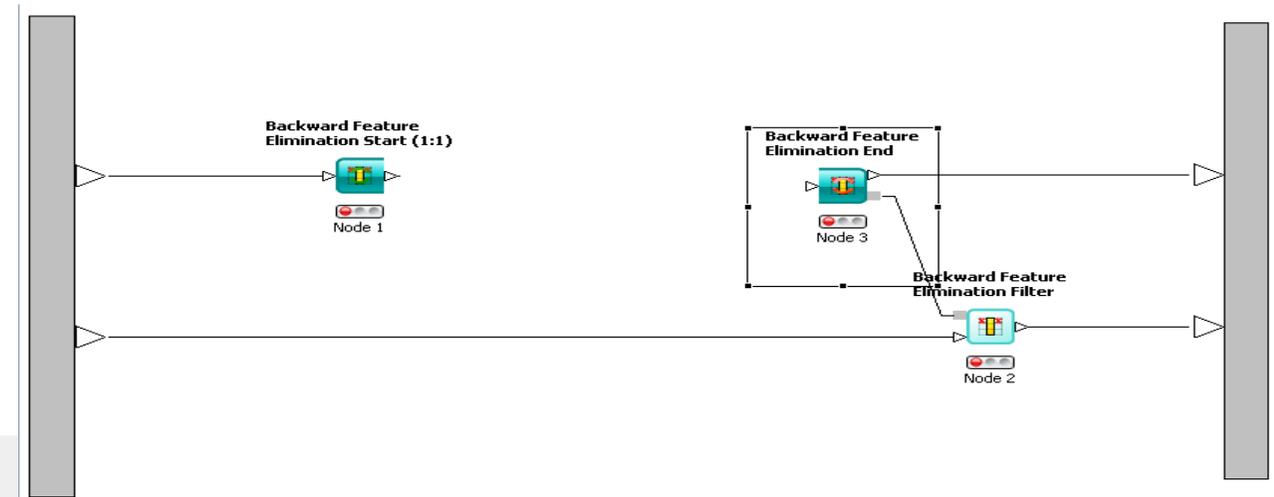
Looping facilities- Basics

- Database
 - Database Looping
- Loop Support
 - Cross Validation
 - X-Partitioner
 - X-Aggregator
 - Feature Selection
 - Backward Feature Elimination Start (1:1)
 - Backward Feature Elimination Start (2:2)
 - Backward Feature Elimination End
 - Backward Feature Elimination Filter
- Counting Loop Start
- Generic Loop Start
- TableRow To Variable Loop Start
- Loop End
- Variable Condition Loop End
- Variable Based File Reader
- Inject Variables (Data)
- Inject Variables (Database)
- Extract Variables (Data)
- Extract Variables (Database)
- TableRow To Variable
- Variable To TableRow
- Variable To TableColumn
- Interval Loop Start
- Meta
 - Loop x-times
 - Variables Loop (Data)
 - Variables Loop (Database)
- Schrödinger
 - Tools
 - Row Iterator Loop Start

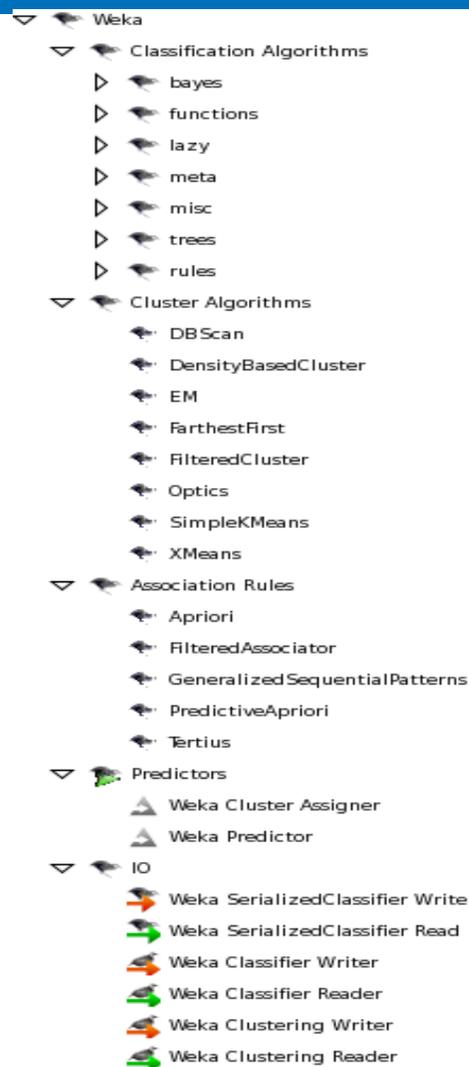
- Loop start ... Loop end
- Inject and extract variables
- TableRow/Column to and from variables
- Prebuilt protocols

- Schrödinger node: Row iterator loop start ▶

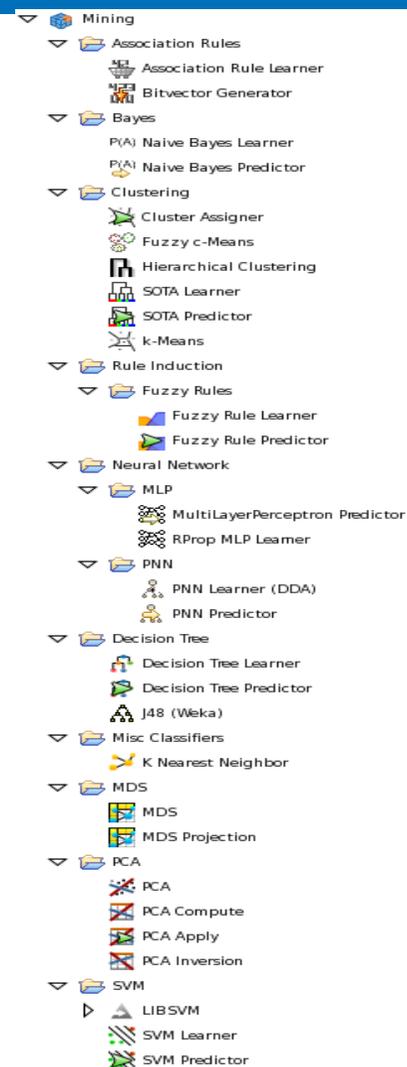
- Meta
 - Feature Elimination
 - Iterate List of Files
 - Loop x-times
 - Variables Loop (Data)
 - Variables Loop (Database)
 - X-Validation
 - Simple Preprocessing



Model building nodes



+ Future Canvas nodes
(already some prototypes)



- Edit variables and advanced looping functionalities
- Hilite functionalities
- Database nodes
- Miscellaneous useful nodes

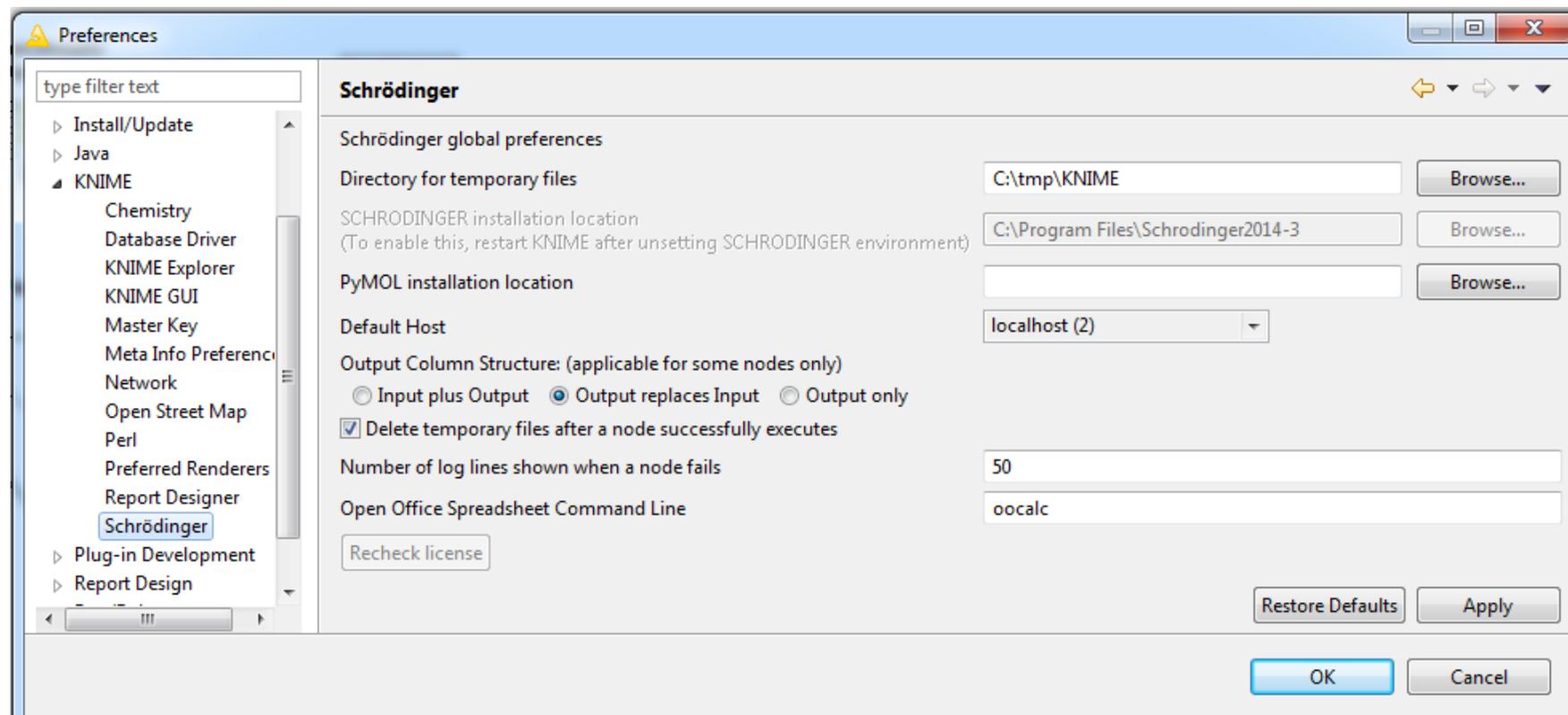


- Schrödinger preferences
- Start-up script options
- Access to the flow variables

Schrödinger Preferences

- A specific scratch directory can be specified for Schrödinger nodes
- Delete temporary files after a node successfully executes

Toggle off to run the calculation through the command line again



Start-up script options

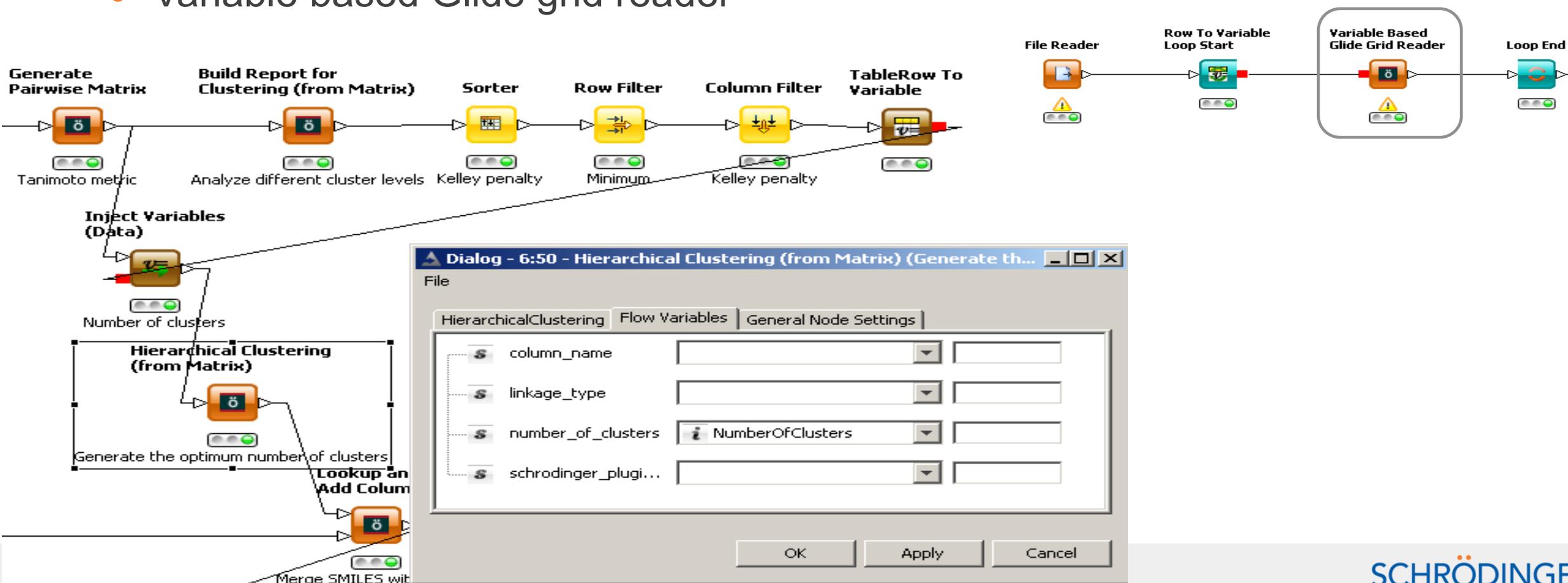
To pass user/machine/OS-specific parameters

-maxHeap	Maximum heap size	eg 2048 for 2G
-maxThreads	Maximum working threads	
-tempDir	Schrödinger extensions temporary directory	
-defaultHost	Default host	
-deleteTempFiles true/false	Delete temporary files on or off.	
-ooCmd <value>	Excel / Open Office Spreadsheet command	
eg oocalc		
or C:\Program Files (x86)\Microsoft Office\Office12\EXCEL.EXE		

And more (see `knife -h` message)

Access to the flow variables

- Access to the flow variables in the Flow variable tab including the Chemistry external tools nodes (using %flow_n%)
- Variable based Glide grid reader





- Chemistry tool nodes
- Python nodes
- Row iterator loop start
- Look up and add vs. Joiner node
- Miscellaneous nodes: Compare ligands, Set molecule title, Get PDB

Chemistry external tool nodes

%\", where <n> is 1, 2, or 3 for specifying the flow variables flow_<n>, the string \"%row_id%\" for specifying the row id (only for each row), and \"%output_1%\" for specifying the output file)'. Buttons for 'OK', 'Apply', and 'Cancel' are at the bottom."/>

Dialog - 5:42 - Chemistry External Tool 1:1 (Parse the log file)

File

ChemExternalTool11 | Flow Variables | General Node Settings

Output Column Structure

Input plus Output

Output replaces Input

Output only

Column containing input (%input_1%): Log Log

Run command line for each input row

Output Type (%output_1%): Text

Output Column Name: Text

Command line(s):

```
grep "high, medium" %input_1% > %output_1%
sort %output_1% > tmp.txt
uniq tmp.txt > %output_1%
rm tmp.txt
```

(Use the string '%input_1%' for specifying the input file,
the string '%flow_<n>%', where <n> is 1, 2, or 3 for specifying the flow variables flow_<n>,
the string '%row_id%' for specifying the row id (only for each row),
and '%output_1%' for specifying the output file)

OK Apply Cancel

- Input/output types:
 - Maestro, SD, mol2, Smiles
 - Double, Integer
 - String, Text
 - Sequence, alignment
 - FingerPrint, Canvas Matrix
 - Phase Hypothesis, Glide Grid

Python nodes

Dialog - 2:359 - Python Script 1:1 (Distance, ASL from columns)

File

Script Flow Variables General Node Settings

Script

```
import os, random, string, subprocess, sys
# Read in the input table
iterator = inData[0].iterator()
while iterator.hasNext():
    row = iterator.next()
    mae_ct = row.getCell(0)
    asl1 = row.getCell(1).value
    asl2 = row.getCell(2).value
# Loop over structures in table (single entries in cell only)
for st in mae_ct.getStructureReader():
    [atom1]= structureutil.evaluate_asl(st, asl1)
    [atom2]= structureutil.evaluate_asl(st, asl2)
    distance = st.measure(atom1,atom2)
    print "distance = "+str(distance)
# Store the distance in the CTs
st.property['r_user_distance']= distance
st.property['s_user_asl1']= asl1
st.property['s_user_asl2']= asl2
# Create the output table
newCell = MaestroCell()
newCell.setToStructure(st)
newRow = AppendedColumnRow(row, [ newCell ])
newRow.colNames = ["New_CT"]
outContainer[0].addRowToTable(newRow)
```

OK

Apply

Cancel

- Input/output connectors: 0:1, 1:1, 1:2, 2:2
- Schrödinger's APIs
- Possibility to include third party APIs

Row iterator loop start

Read table - 4:58 - Table Reader (Se...)

File

Spec - Columns: 2 | Properties

Table "default" - Rows: 3

Row ID	group	CT
Row1	0	#CTs: 10
Row2	1	#CTs: 10
Row3	2	#CTs: 5

Row Iterator
Loop Start

Ungroup MAE

Row Filter

Loop End

Only the second structure

Input with expanded column in Sequence, Alignme...

File

Table "default" - Rows: 5 | Spec - Columns: 2 | Properties

Row ID	group	CT
Row1	2	Molecule: 1wun_lig_ref #atoms:...
Row2	2	Molecule: 2brn_lig_ref #atoms: 46
Row3	2	Molecule: 2fdp_c_lig_ref #atom...
Row4	2	Molecule: 2itw_a_lig_ref #atoms...
Row5	2	Molecule: 2vgp_a_lig_ref #atom...

Dialog - 4:64:7 - Row Filter (Only the second structure)

File

Filter Criteria | Flow Variables | General Node Settings

Set filter parameter:

Row number range:

first row number: 2

to the end of the table

last row number: 2

include rows by attribute value

exclude rows by attribute value

include rows by number

exclude rows by number

include rows by row ID

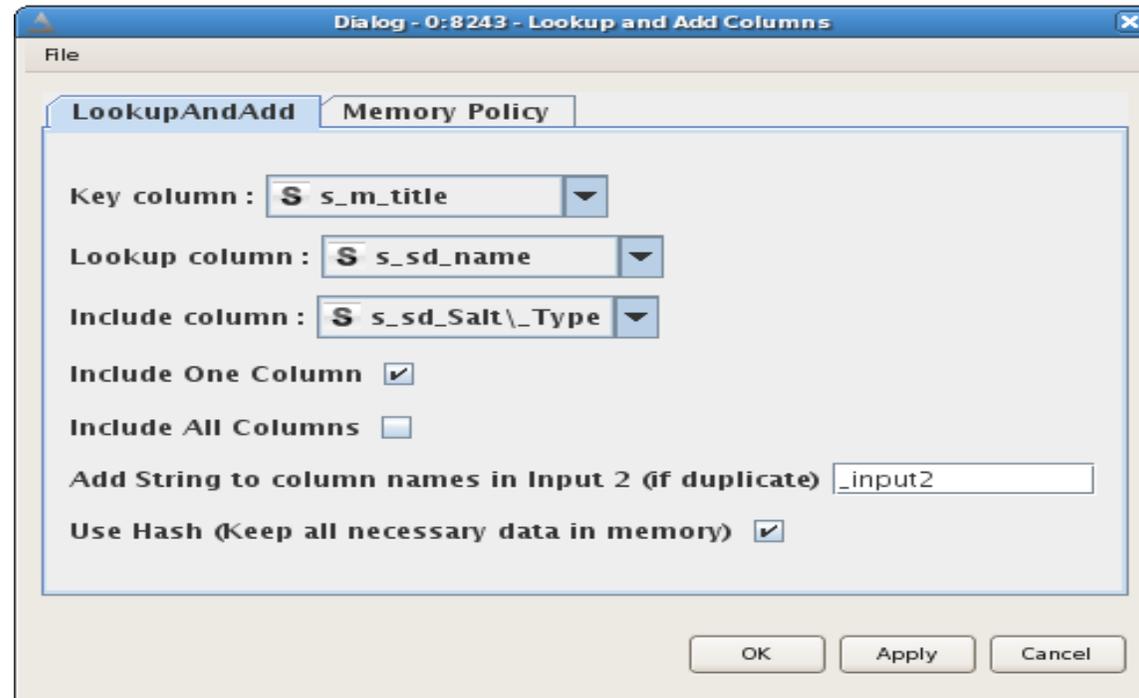
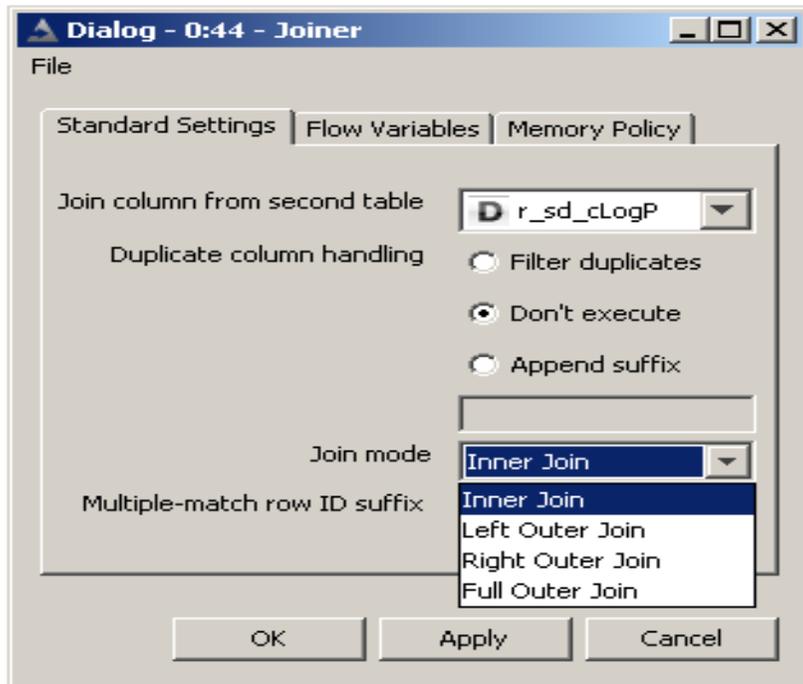
exclude rows by row ID

OK Apply Cancel

Look up and add vs. Joiner node

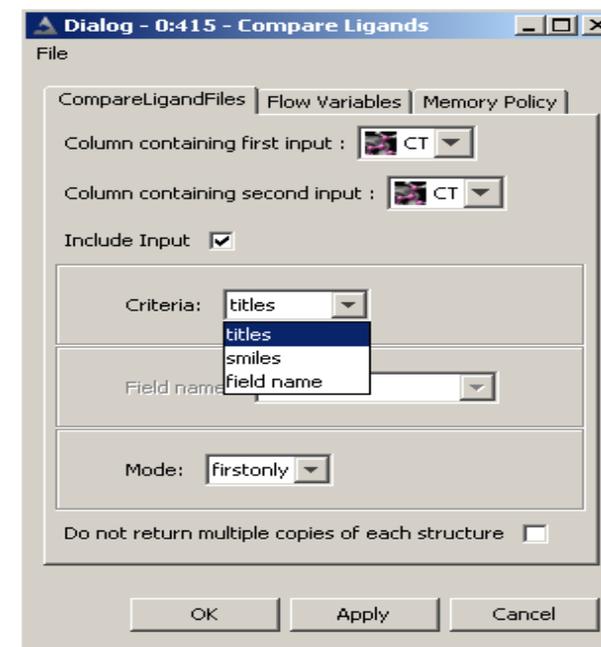
- Take advantage only 1 column, concatenate columns

The Joiner node is the easiest way to concatenate columns when the table have the same number of rows and same rowIDs.



Miscellaneous nodes

- Get PDB: easy way to get one or several structures
use the | symbol as a delimiter for the list of codes
- Set molecule title
- Compare ligands: the modes are First only, both, either





- Simple workflow examples
- Workflow development support for customers
- Automatic protein preparation
- Scientifically relevant application of the workflow examples
- Interactive work with Knime using the HiLite functionalities
- Use a workflow again

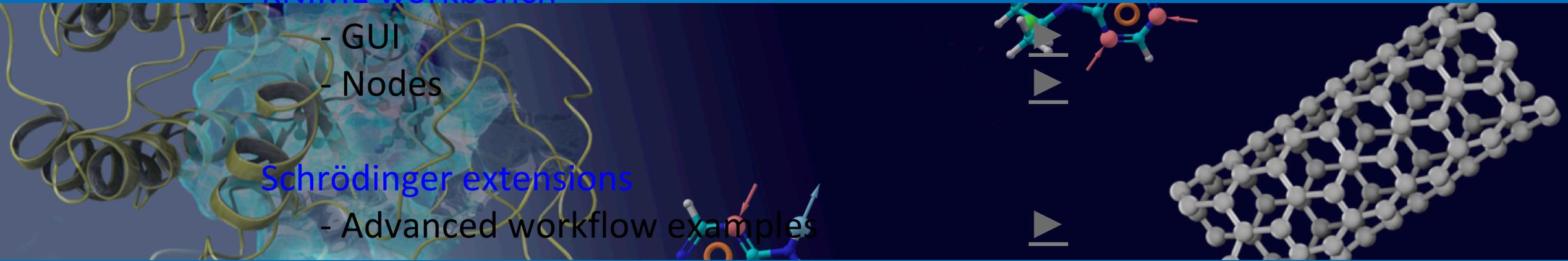
Advanced functionalities

KNIME workbench

- GUI
- Nodes

Schrödinger extensions

- Advanced workflow examples



◀ Intermediate

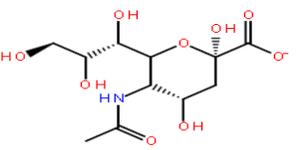
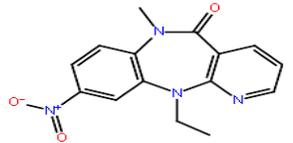
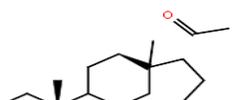


- Report designer
- Global variables
- Batch execution
- Tips and tricks

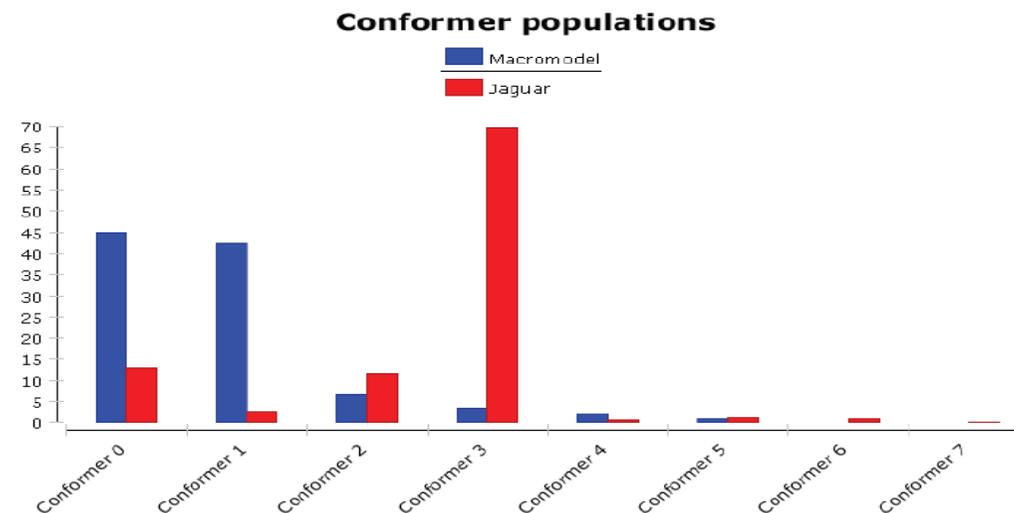
Report designer

- From knime.com but free of charge. Included in our distribution
- Include To report node(s) in the workflow (can't be in metanodes) and switch to the Report designer mode

BIRT Report Viewer

Ligand	Complex	Ligand origin	Binding site	Mutations
	1a4q	1nsc	ligand A:DPC2	No
	1buh	1dm2	residues A:18,A:80,A:314	No
	1c1c	1rth	ligand Z:UNK999	A:102,A:227,A:234,B:102,B:234
	1dba	1dbb	ligand _:STR1	H:104

Isomenthone conformational analysis



Row ID	Jaguar			MacroModel		
	Relative Energy	Ring conformation	Boltzmann population	Relative Energy	Ring conformation	Boltzmann population
Conformer 3	0.0	-104.2	69.9	6.32	-104.3	3.6
Conformer 4	11.65	-80.0	0.7	7.67	-85.9	2.1
Conformer 5	10.29	-68.9	1.1	9.9	-82.7	0.8
Conformer 7	15.96	-18.4	0.1	18.55	-20.4	0.0
Conformer 6	10.55	-18.3	1.0	17.95	-21.3	0.0
Conformer 0	4.17	-1.1	13.1	0.0	-5.3	44.8
Conformer 1	8.09	1.3	2.7	0.15	-3.1	42.2
Conformer 2	4.52	6.5	11.4	4.82	1.3	6.5

Report designer- template mode

The screenshot displays the KNIME Report Designer interface in template mode. The main window shows a report preview with the following content:

3: Virtual screening Workflow executed

1 View Report in Web Viewer
2 View Report as DOC
3 View Report as HTML
4 View Report as PDF
5 View Report as POSTSCRIPT
6 View Report as PPT
7 View Report as XLS

<H1><CENTER>Virt...</H1>

PDB ID
[BestRepresentative]
Footer Row

<H2>Hit list</H2>

Smiles	Title	Glide score
[X]	[Title]	[r_i_docking_score]
Footer Row		

<H2>PDB struct...</H2>

Smiles	PDB ID	Resolution
[X]	[s_pdb_PDB_ID_input]	[r_pdb_PDB_RESOLU...]

Property Editor

Properties

General

Description

Comments

User Properties

Named Expressions

Resources

Event Handler

Advanced

Author: []

Created by: Eclipse BIRT Designer Version 2.3.2.r232_20090202 Build <2.3.2.v20090218-0730>

Path: C:_xknime-example\mainKNIMEworkspace\Workshop materials\2010 UGM\3- HTVS\Virtual screening- Wc

Title: []

Themes: None

Report Orientation: Left To Right

Display Name: []

Thumbnail: /templates/blank_report.gif

Layout Preference: Auto Layout Fixed Layout

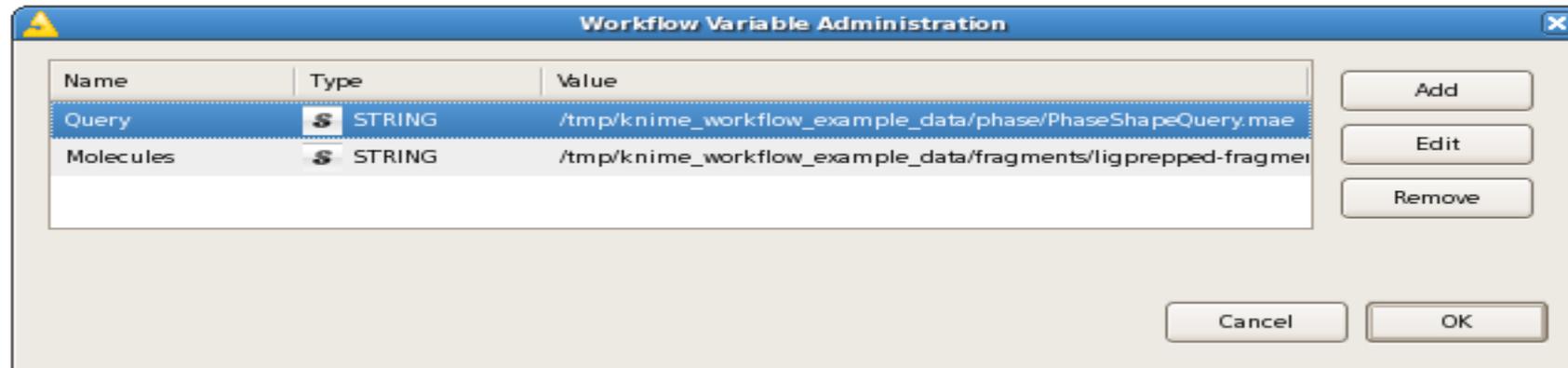
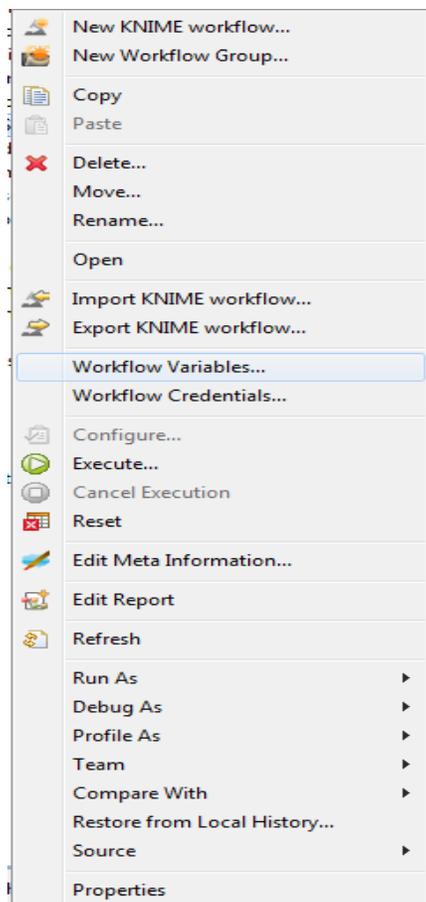
Report designer- Canvas 2D renderer

The structures can be shown in a report using Canvas 2D renderer using the following procedure:

- 1. In the workflow, add a MAE-to-smiles node and a To report node.
- 2. In Reporting mode, in the Layout tab, add a table to the report (drag and drop from the Data set view).
- 3. Insert in the "[smiles]" cell (Table- detail row) an Image widget from the Report Items list.
- 4. Configure the widget (using "Edit" on the widget), select "Dynamic image", and press "Select Image Data..." to select the source column (which should be the Smiles column). Delete "[smiles]" if you want just the image and no SMILES. You may want to alter the size of the cell by dragging the border vertically and horizontally if necessary.
- 5. Change the size of the image to something like 300x300, which is done by editing the Data set view (right click -> Edit -> Parameters), and changing (or creating new Parameters typed as integer if they don't exist yet) the knime-image-height and knime-image-width parameters.
- 6. Check the view in the Preview tab

Global variables

- In the Workflow project list, right-click on the workflow, under Workflow variables



Batch execution

- `$SCHRODINGER/knime -batch -reset -nosplash -nosave`
 -workflowFile=<path>/<wkf>.zip or **-workflowDir**=<path>/<workspace>/<wkf>
- Alter some settings **-option=nodeNumber,valueName,value,type**
 -option=7,filename,"/tmp/new-molprops.csv",String (int, double or String)

Find the node number in the configuration panel header (add the metanode numbers)

eg 123/456/78 for the node 78 in the metanode 456 in the metanode 123

Find the option name in the workspace directory: <workflow>/node_name(#7)/node.xml eg:

```
<config key="DataURL">
```

```
<entry key="array-size" type="xint" value="1" />
```

```
<entry key="0" type="xstring" value="/C:/serotonin_unique.sdf" />
```

```
-option=2,DataURL\0,"file:/tmp/new-input.mae",String
```

When the input is an array

- Pass some variables: **-workflow.variable=name,value,type** (int, double or String)
- Workflows can be run from Maestro using a simple Python script wrapper

Tips and tricks

- Rearrange the panels
- Workflow Meta-Infos
- Try to open a workflow modified with a newer version of KNIME alter the 2 following lines of the file

```
<workspace>/<workflow>/workflow.knime:
```

```
<entry key="created_by" type="xstring" value="2.0.3.0021120"/>
```

```
<entry key="version" type="xstring" value="2.0.0"/>
```



- Edit variables and advanced looping functionalities
- HiLite functionalities
- Database nodes
- Miscellaneous useful nodes

Edit variables and advanced looping functionalities



- Extract variable (data) and Inject variable (data)
- TableRow to Variable (use the first row), Variable to TableRow and Variable to TableColumn

Hilite functionalities

- HiLite filter and HiLite collector nodes
- Color, Size and Shape Manager/Appender nodes

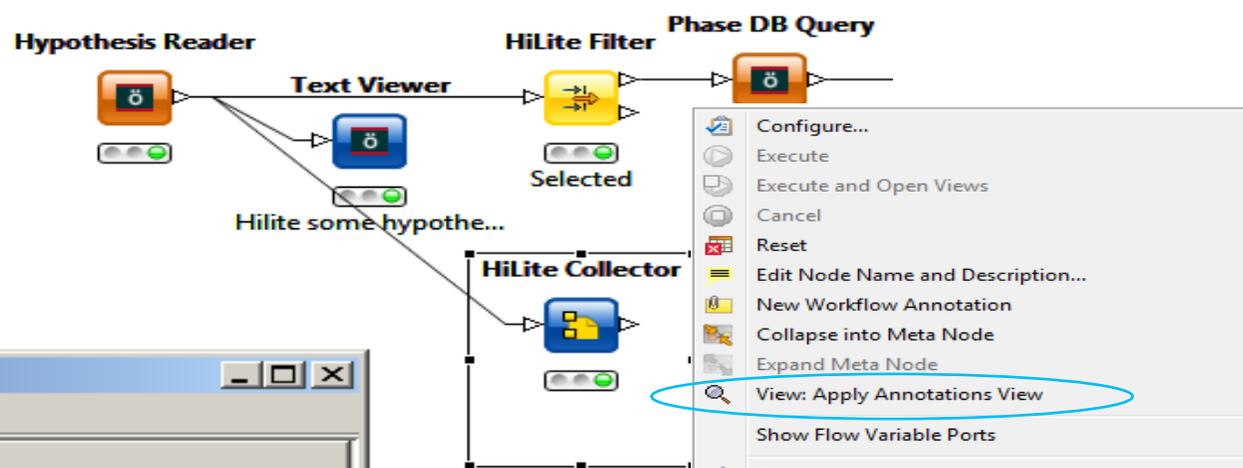
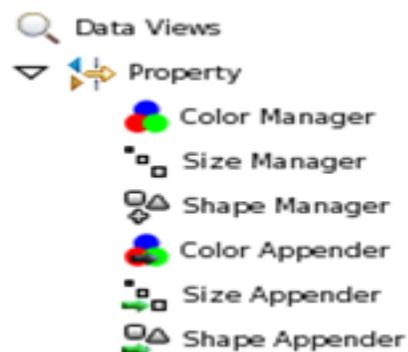


Table View - 2:8240 - Text Viewer (Hilite some hypotheses)

File Hilite Navigation View Output

Row ID	hypothesis
Row0	Hypothesis: "AAADPR_1005" From: "/tmp/knime_workflow_example_data/PhaseHypothes...
Row1	Hypothesis: "AAADPR_1109" From: "/tmp/knime_workflow_example_data/PhaseHypothes...
Row2	Hypothesis: "AAADPR_242" From: "/tmp/knime_workflow_example_data/PhaseHypotheses"
Row3	Hypothesis: "AAADPR_552" From: "/tmp/knime_workflow_example_data/PhaseHypotheses"
Row4	Hypothesis: "AAADPR_964" From: "/tmp/knime_workflow_example_data/PhaseHypotheses"
Row5	Hypothesis: "AAADPR_981" From: "/tmp/knime_workflow_example_data/PhaseHypotheses"
Row6	Hypothesis: "AAADPR_982" From: "/tmp/knime_workflow_example_data/PhaseHypotheses"
Row7	Hypothesis: "AAADPR_983" From: "/tmp/knime_workflow_example_data/PhaseHypotheses"
Row8	Hypothesis: "AAADPR_984" From: "/tmp/knime_workflow_example_data/PhaseHypotheses"
Row9	Hypothesis: "AAADPR_998" From: "/tmp/knime_workflow_example_data/PhaseHypotheses"
Row10	Hypothesis: "AAADPR_999" From: "/tmp/knime_workflow_example_data/PhaseHypotheses"
Row11	Hypothesis: "AAADPR_1000" From: "/tmp/knime_workflow_example_data/PhaseHypotheses"
Row12	Hypothesis: "AAADPR_1001" From: "/tmp/knime_workflow_example_data/PhaseHypotheses"

Hilite Selected
Unhilite Selected
Clear Hilite
Filter

Apply Annotations View - 0:8253 - HiLite Collector

File Hilite

Append Annotation

Scaffold 1 Apply New Column

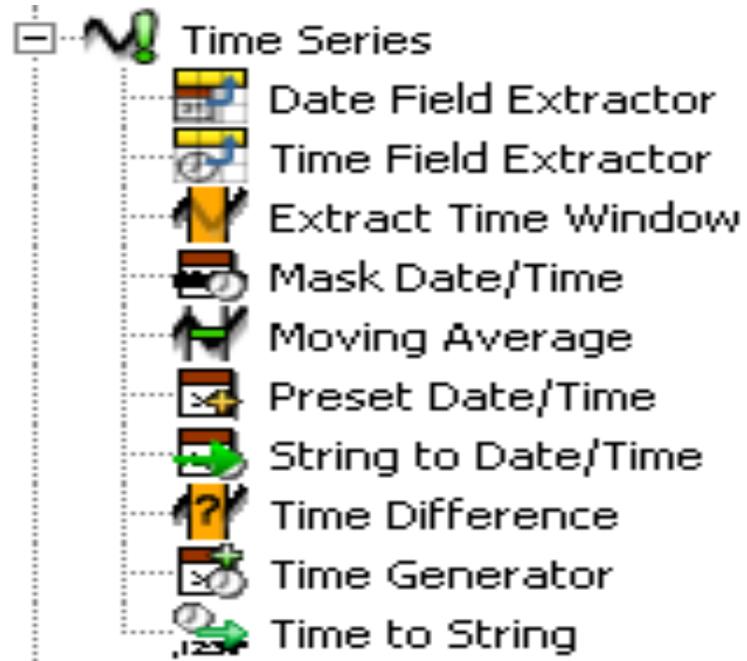
Row ID	S Anno #0	S Anno #1
Row9	Active	Scaffold 1
Row7	Active	Scaffold 1
Row1	Active	Scaffold 1

Database nodes

-  Database
 -  Database Reader
 -  Database Connector
 -  Database Looping
 -  Database Row Filter
 -  Database Query
 -  Database Column Filter
 -  Database Connection Writer
 -  Database Writer
 -  Database Connection Reader

See simple examples (not on the Workflow page yet)

Time series support



- See simple examples (not on the Workflow page yet)

Miscellaneous nodes: Cell splitter, Numeric binner

- Reference row filter, Reference column filter, Nominal value row filter
- Missing values
- Create collection column and Split collection
- Text manipulation: String replacer, Case converter, Cell splitter
- Row sampling, Partitioning, Shuffle
- Numeric binner



- KNIME workflow page
- Workflow development support for customers
- Workflow example presentation

Cheminformatics

- [Substructure Search](#)
- Clustering, diversity selection, similarity search
- [Database analysis](#)
- [Maximum Common Substructure](#)

Docking and post-processing

- [Protein preparation and Glide grid generation](#)
- Docking and scoring, Virtual screening, Ensemble docking, Induced Fit Docking
- [Loop over docking parameters](#)
- [Validate docking parameters](#)

Pharmacophore modeling

- [Phase Shape screening](#)
- Phase hypothesis identification
- [Phase database screening](#)

Molecular Mechanics

- [Compare conformational search methods](#)

Quantum mechanics

- [Conformational search and QM optimization](#)
Using the Report designer

Homology modeling

- Model building and refinement

Library design

- [Library enumeration](#)
including a [Run Maestro 1:1 prototype](#)

Real World Examples

- [Vendor database preparation](#)

General tools

- Python script node use-cases
including a [Run PyMOL prototype](#)
- Chemistry external tool node use-cases
- Run maestro command node use-cases
- Output column structure option philosophy

KNIME workbench

- [Workflows in the current workspace](#)

KNIME workbench- looper

- Group Looper

Simplest, **most exciting**, **new** and improved workflows

Workflow development support for customers

Combine or expand the workflow examples

- Hierarchical clustering and diverse compounds from each cluster

Waiting for new nodes to be developed

- CombiGlide library enumeration, MacroModel coordinate scan (now available)
- PCA on per residue interactions (Chemistry external tool node)
- Distance measurement in protein and run script in Maestro, descriptor calculation, create protein mutants (Python script node)

Specific workflows

- Various MacroModel protocols using the Python node for accessing advanced functionalities (eg constraints)
- Prime MM-GB/SA on a set of complexes (ligand detection, flexible residues)
- Simplifying compound docking with KNIME, Dr. Robert Happel, Boehringer Ingelheim, Vienna
<http://www.schrodinger.com/seminarprior/19/26/>
- Cris Guimaraes MM-GB/SA paper reproduction and improvements
<http://www.schrodinger.com/Download.php?type=seminarentry&type2=slides&ident=105>
- Protein preparation protocol

Real World Case Study: Binding Site Clustering and Ensemble Docking

Chem Biol Drug Des 2012; 80: 182–193

© 2012 John Wiley & Sons A/S
doi: 10.1111/j.1747-0285.2012.01966.x

Research Article

Generation of Receptor Structural Ensembles for Virtual Screening Using Binding Site Shape Analysis and Clustering

David J. Osguthorpe¹, Woody Sherman² and Arnold T. Hagler^{1,3,*}

Virtual screening is an important part of computer-aided drug design, with many reviews (1–3) and successful applications reported (4–7) in the literature. Although ligand-based methods have been shown to yield high database enrichments in virtual screening (8–10), use of

¹Shifa Biomedical, 1 Great Valley Parkway, Suite 8, Malvern, PA

THE JOURNAL OF
PHYSICAL CHEMISTRY B

Article
pubs.acs.org/JPCB

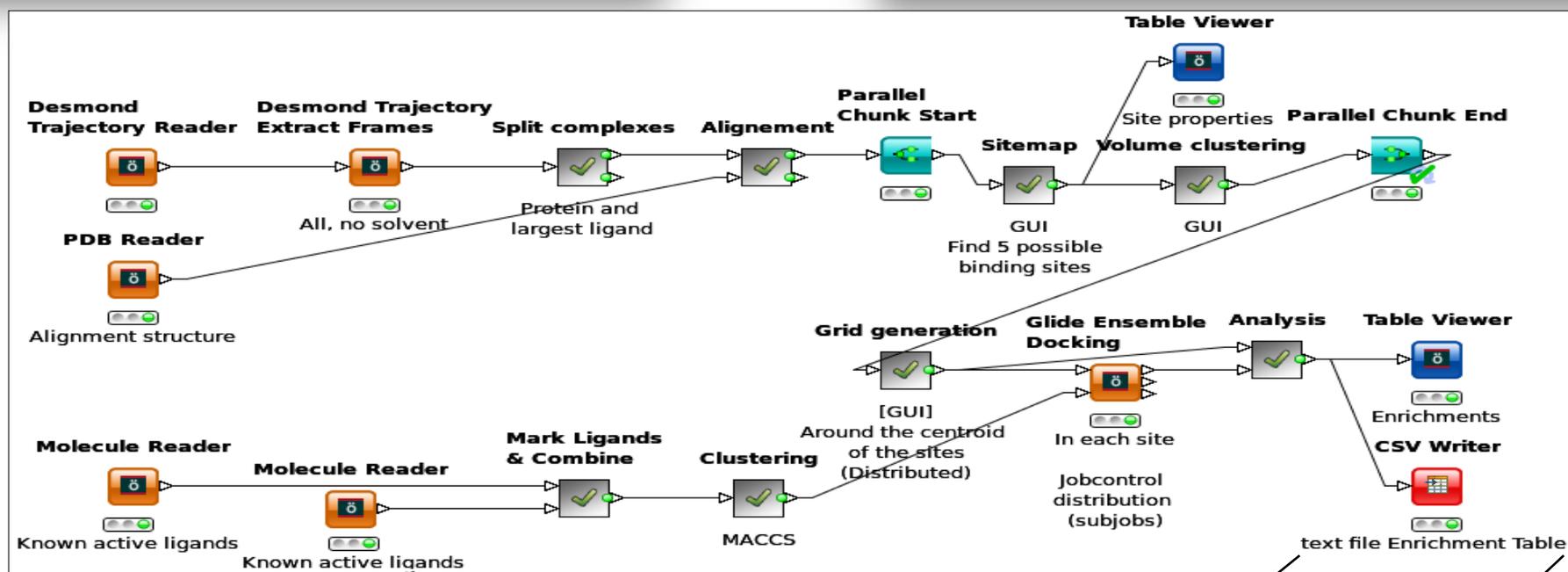
Exploring Protein Flexibility: Incorporating Structural Ensembles From Crystal Structures and Simulation into Virtual Screening Protocols

David J. Osguthorpe,[†] Woody Sherman,[‡] and Arnold T. Hagler^{*,†,§}

[†]Shifa Biomedical, 1 Great Valley Parkway, Suite 8, Malvern, Pennsylvania 19355, United States

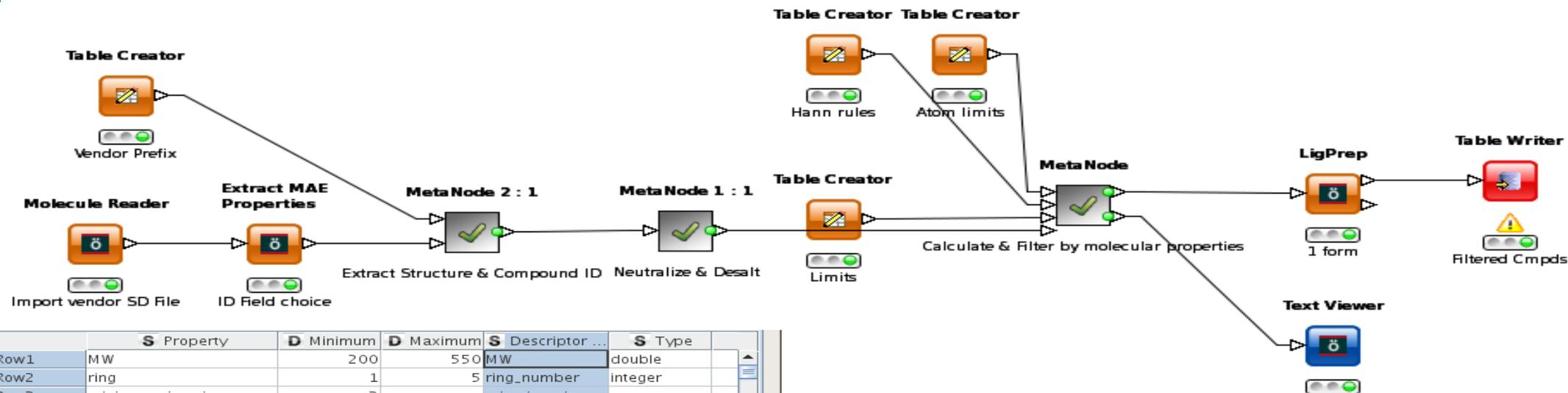
[‡]Schrödinger, Inc., 120 West 45th Street, 17th Floor, New York, New York 10036, United States

[§]Department of Chemistry, University of Massachusetts, 701 Lederle Graduate Research Tower, 710 North Pleasant Street, Amherst, Massachusetts 01003-9336, United States

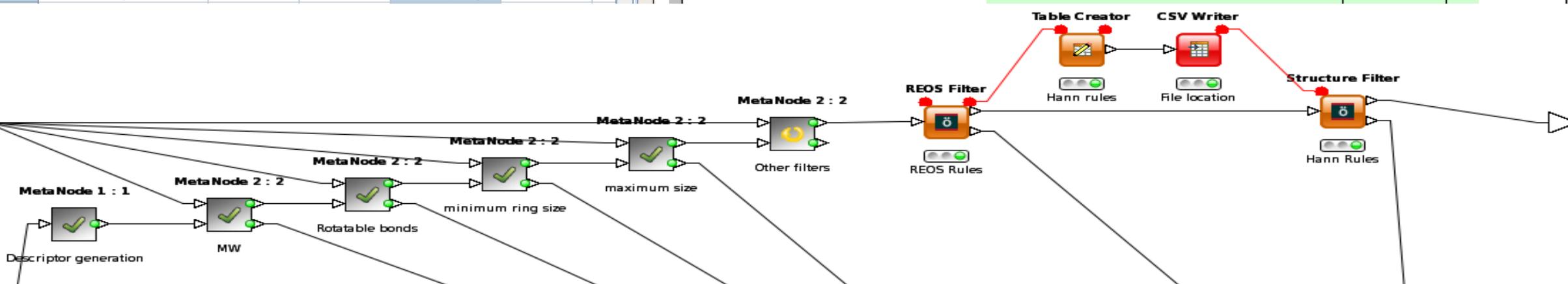
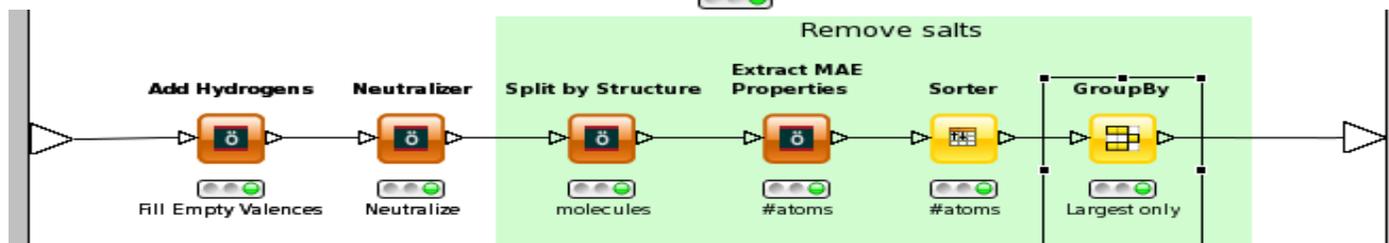


File	Hilite	Navigation	View	Output				
Row ID	S	Sitemap	D AUC	D ef 1%	D 1%	D ef 4%	D 4%	D Sitescore
activ#6		Frame 120_site_1		23.72		8.372		1.175
activ#0		Frame 0_site_1		22.875		9.65		1.244
activ#3		Frame 40_site_1		15.547		9.893		1.219
activ#8		Frame 160_site_5		6.949		3.786		0.636
activ#2		Frame 0_site_4		2.94		0.715		0.878
activ#4		Frame 80_site_3		2.819		1.047		0.66
activ#1		"activ#2" (5/9)		0		0		0.686
activ#5		Frame 80_site_5		0		0.687		0.559
activ#7		Frame 160_site_3		0		1.737		0.794

Real life applications...



	S Property	D Minimum	D Maximum	S Descriptor ...	S Type
Row1	MW	200	550	MW	double
Row2	ring	1	5	ring_number	integer
Row3	minimum ring size	3		min_ring_size	> =
Row4	maximum ring size	8		max_ring_size	< =
Row5	unbranched	0	6	longest_unbr...	integer
Row6	hetero atoms	1	14	hetero_atoms	integer
Row7	heavy atoms	10	100	i_ligfilter_Num...	integer
Row8	hetero/heavy atom ratio	0.1	0.5	hetero/heavy_...	double
Row9	fused rings	0	3	largest_fused...	integer
Row10	chiral atoms	0	21	i_ligfilter_Num...	integer
Row11	rot bonds	0	10	RB	integer
Row12	aromatic only	0		aromatic_only	< =



Workflow example presentation

Feel free to request this other presentation including:

- Simple examples
- More advanced examples from the Workflow page
- Scientifically relevant applications

Schrödinger KNIME Extensions

KNIME Extensions Product Manager: Jean-Christophe Mozziconacci
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Vice President of Technology: Volker Eyrich

Main Developer: Ravikiran Kuppuraj
and the PyDev development team

QA: Simon Foucher

Workflow examples: Tanvi Bhola

Technical Support: Katalin Phimister, Pavel Golubkov

Marketing: Jarred Yacob