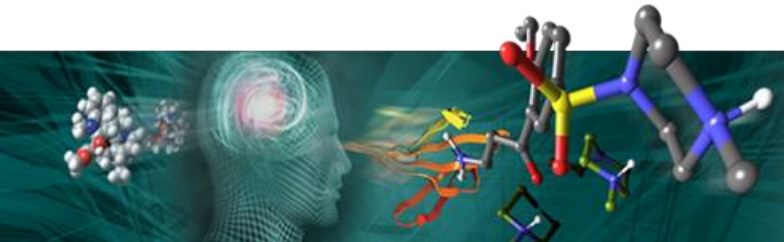
The Schrödinger KNIME extensions

Computational Chemistry and Cheminformatics in a workflow environment

Jean-Christophe Mozziconacci

Volker Eyrich



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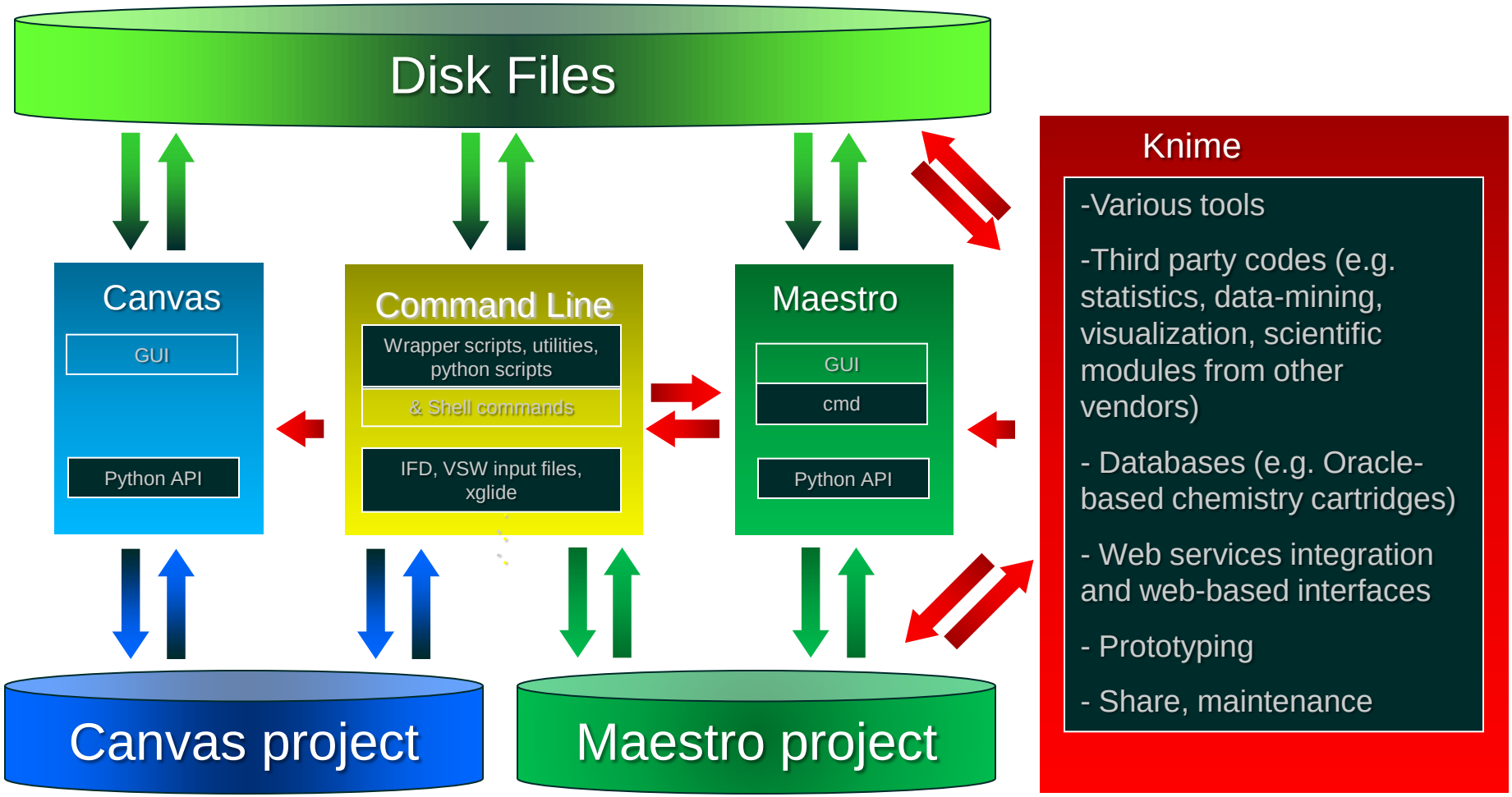
Topics

- Integration options
- What are the Schrödinger extensions?
- Workflow examples
- Roadmap

Integration options



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What are the Schrödinger extensions?

Access to Schrödinger tools via KNIME

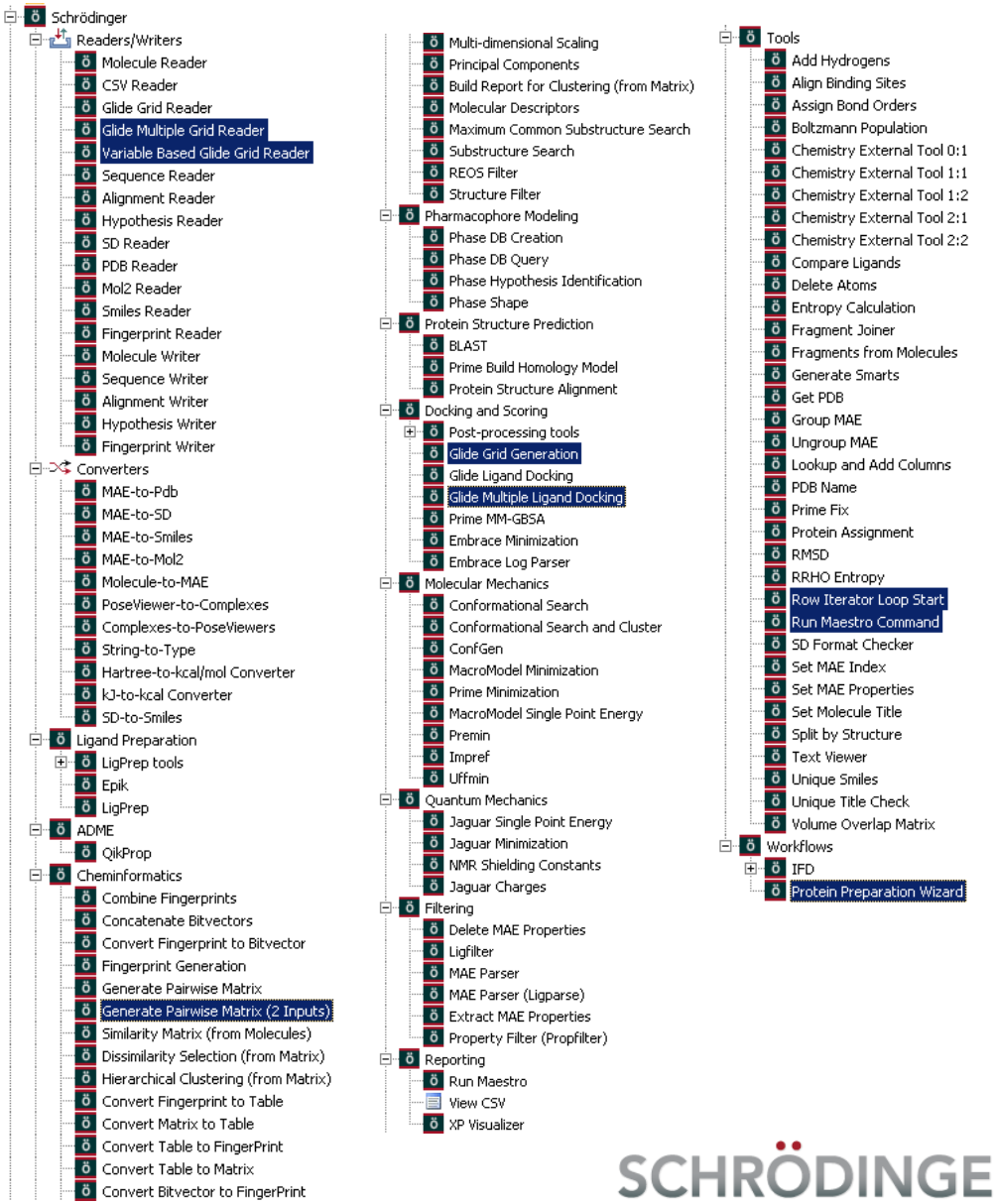
- Modeling and computational chemistry in a workflow environment
- Graphical assembly of workflows
- Generate, manipulate, analyze and visualize chemical data
- Interactive and automated analysis of datasets
- Presentation and communication of results

Access to Schrödinger tools via KNIME

Modeling and computational chemistry in a workflow environment

~140 nodes

- Ligand/protein preparation
- LBDD (cheminformatics, pharmacophore modeling)
- SBDD (Protein structure prediction, docking and scoring)
- Molecular and quantum mechanics



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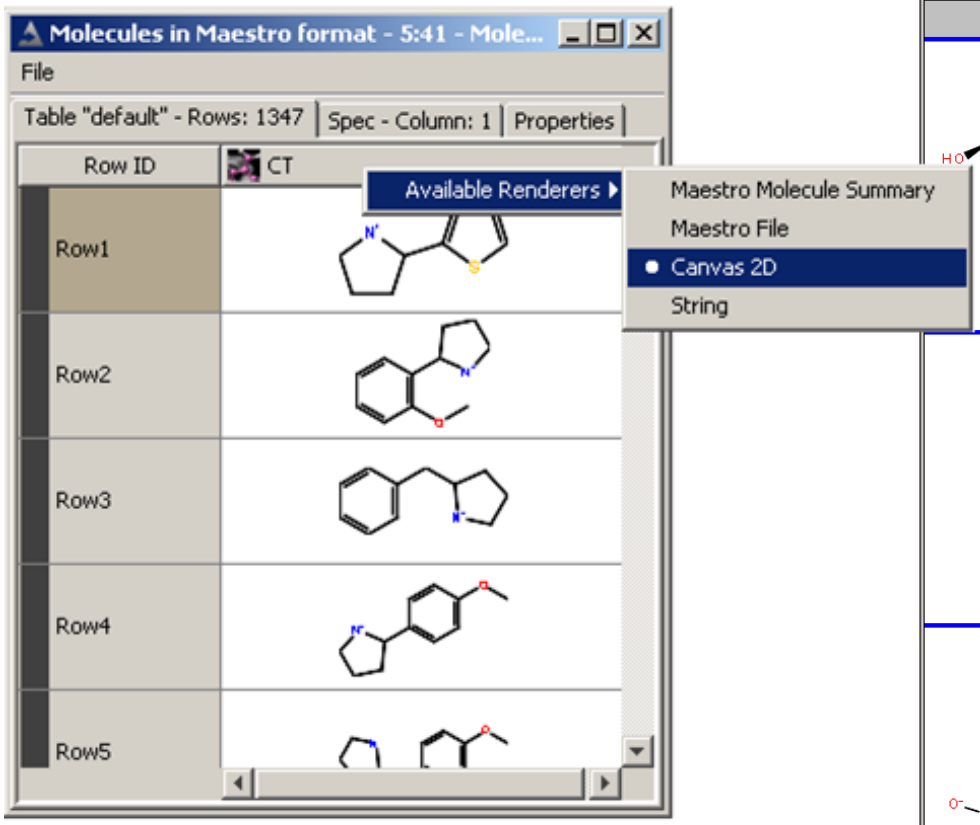
Structure and data manipulation

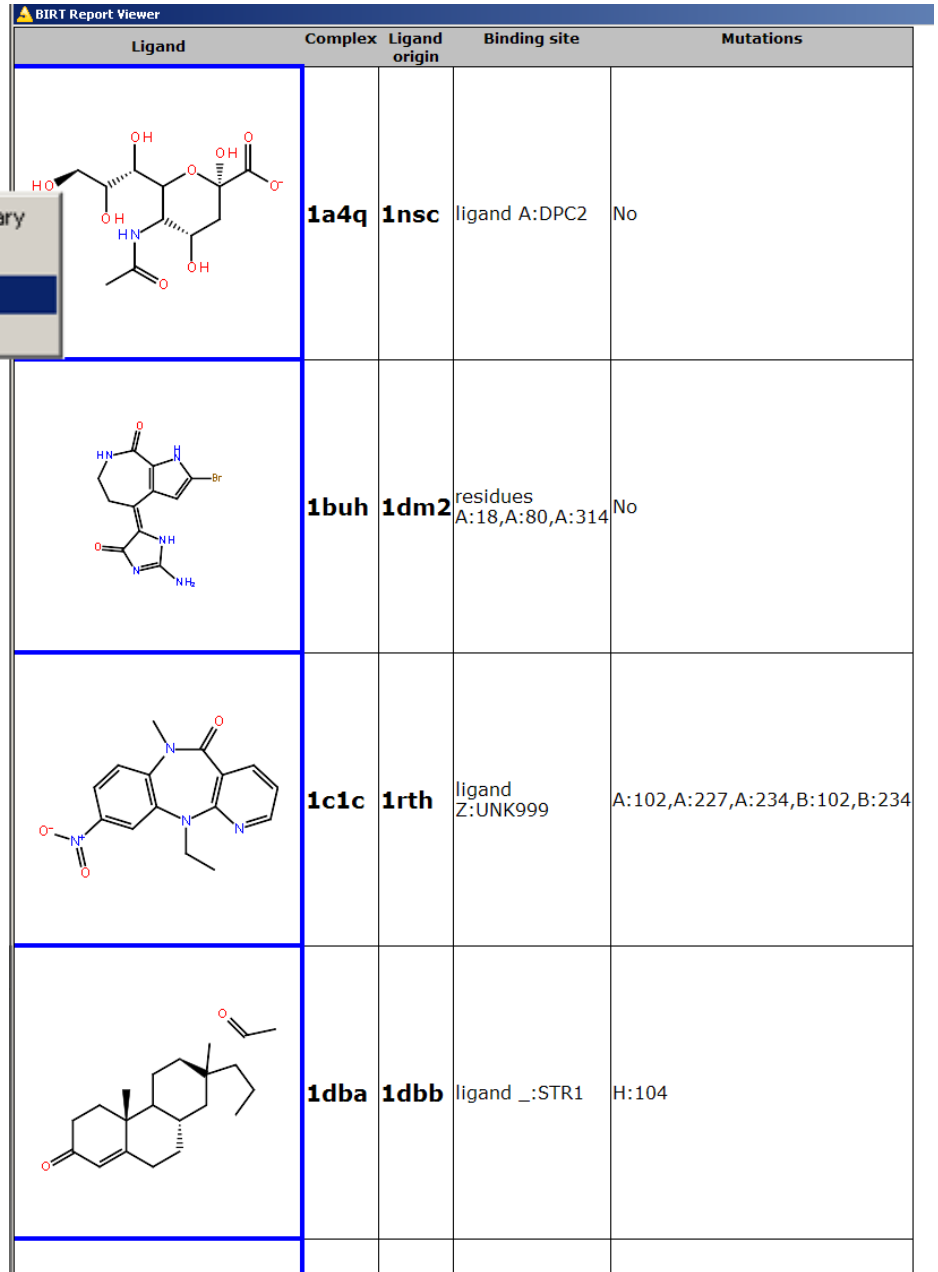
- **Generate, manipulate, analyze and visualize chemical data**
- **Interactive and automated analysis of datasets**
- **Presentation and communication of results**

KNIME nodes

- Readers/Writers, converters, SD format checker,
- Filtering (Ligfilter, MAE parser, Compare ligands)
- Reporting (Text viewer, CSV viewer: OpenOffice/Excel, Run Maestro)
- Grouped structures (Group and Ungroup, Row iterator loop start)
- Structure and data manipulation (RMSD, Look up and add columns, Extract and Set MAE properties, Set MAE index, Split by structure, Delete atoms, Unique smiles, Unique title check, Align binding sites, Volume overlap matrix…)
- Scripting (Run Maestro commands, Python node, Chemistry external tool)

Canvas 2D view and use in the Report designer

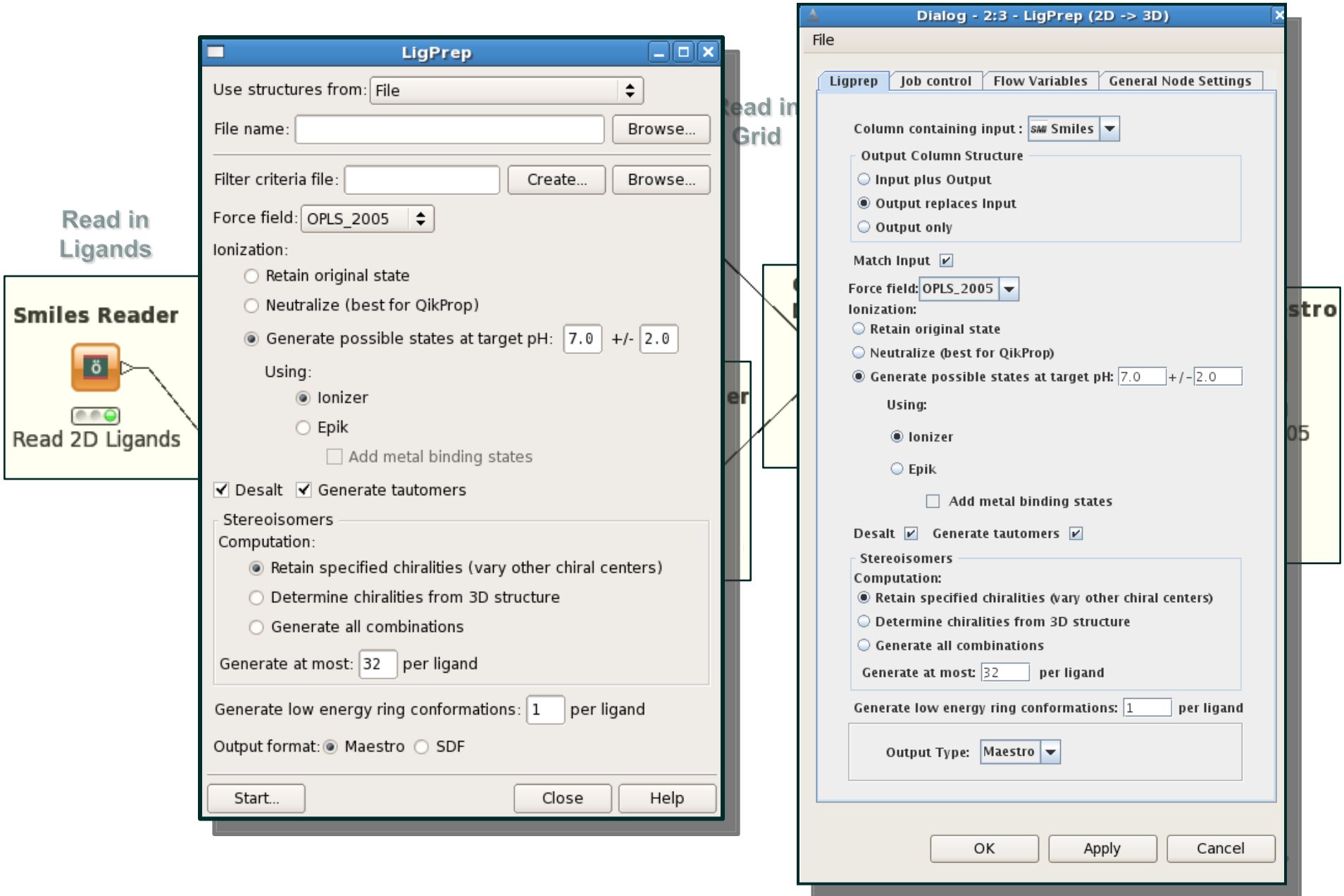




KNIME, Maestro and Canvas

- Launch Maestro or Canvas from KNIME
  - Interactive visualization
  - Run Maestro command scripts
- Launch KNIME from Maestro
  - Through a simple python script
  - Improvements under development
- ‘Visual coherence’ for application GUIs/configuration dialogs

Configuration panel layout – Maestro vs. KNIME



KNIME workflow page http://www.schrodinger.com/knimeworkflows

Select Workflows

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

- Cheminformatics
- Docking / Docking Post-processing
- Molecular Mechanics
- Homology Modeling
- Pharmacophore Modelling
- KNIME Workbench
- General Tools

Check the boxes next to the workflows you wish to download, read the Important Notes, then proceed below to check the Important Notes checkbox and click the Download button.
Note: If you are not already logged in to the site, your selection will be saved and you will be prompted to log in. If you do not already have a logon account, please click here to request one.

Select All | Select Workflows Updated in the Last [30] Days | Reset

Cheminformatics

Select	Description	Author	Updated
☐	**Cluster by Fingerprint**: Cluster structures via binary fingerprints and inspect the clustering statistics to choose a good number of clusters. Generate the clusters, inspect the corresponding list of structures and the clusters' representative molecules. [List of nodes: File Reader, Column Filter, Line Plot, Generate Pairwise Matrix, Row Filter, Build Report for Clustering _from Matrix_, RowID, Fingerprint Generation]	Schrödinger	09/08/2009
☐	**Maximum Common Substructure Search**: 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		09/08/2009

General Tools

Select	Description	Author	Updated
☐	**Ensure molecule title uniqueness**: Ensure unique molecule titles (using the KNIME RowID) in the context of Canvas. [List of nodes: Set Molecule Title, RowID, Similarity Matrix _from Molecules_, Molecule Reader, Extract MAE Properties]	Schrödinger	09/08/2009

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Important Notes

NOTICE: THE WORKFLOWS ON THIS WEB SITE HAVE BEEN GENERATED BY SCHRÖDINGER OR BY USERS OF SCHRÖDINGER SOFTWARE. THE WORKFLOWS ARE PROVIDED FREE OF CHARGE. THE WORKFLOWS ARE PROVIDED "AS IS" WITHOUT WARRANTY OF ANY KIND, AND MAY NOT BE ERROR FREE. SCHRÖDINGER AND THE AUTHORS OF THESE WORKFLOWS DISCLAIM ALL WARRANTIES, EXPRESS OR IMPLIED, INCLUDING WARRANTIES OF MERCHANTABILITY AND FITNESS FOR A PARTICULAR PURPOSE. IN NO EVENT SHALL SCHRÖDINGER OR THE AUTHORS OF THESE WORKFLOWS BE LIABLE FOR SPECIAL, INCIDENTAL OR CONSEQUENTIAL DAMAGES OF ANY KIND.

☑ Include optional example data in the download.

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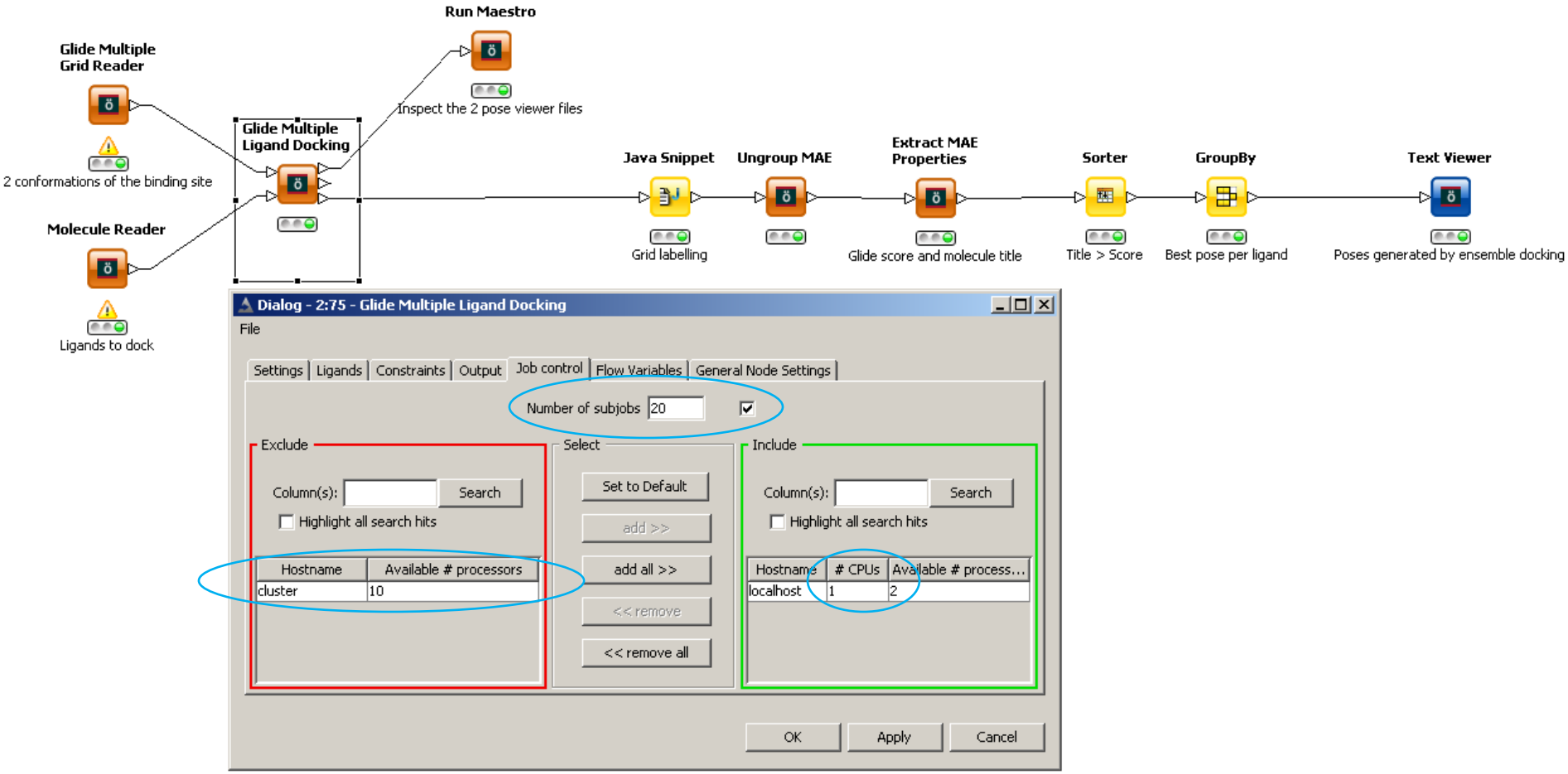
Ensemble docking



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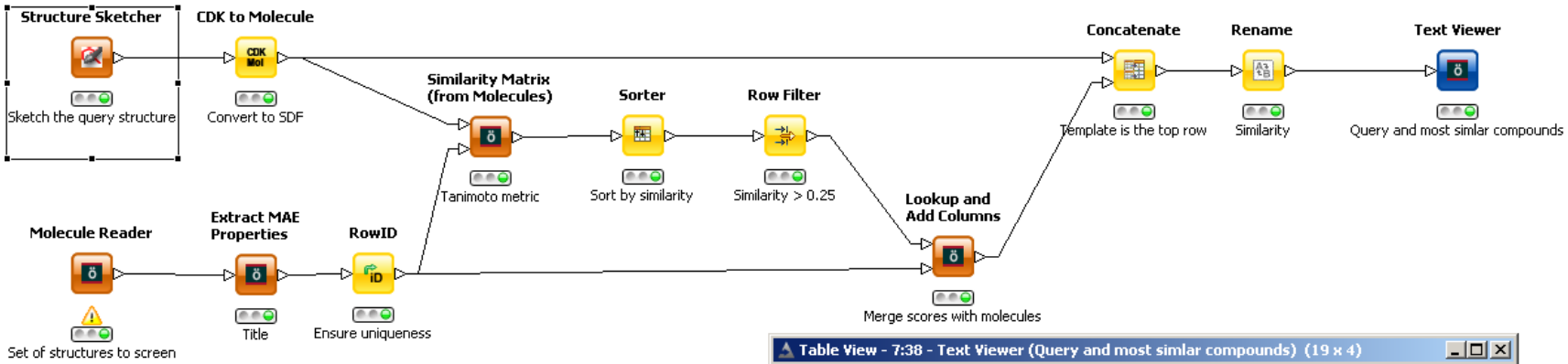
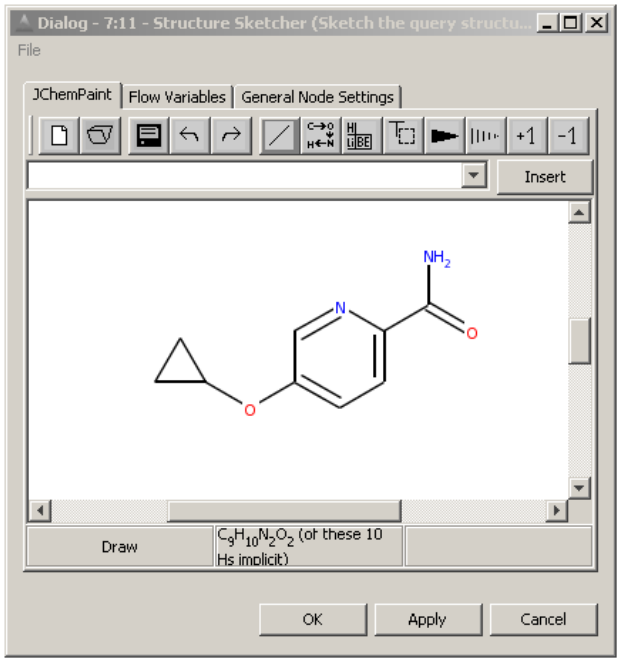
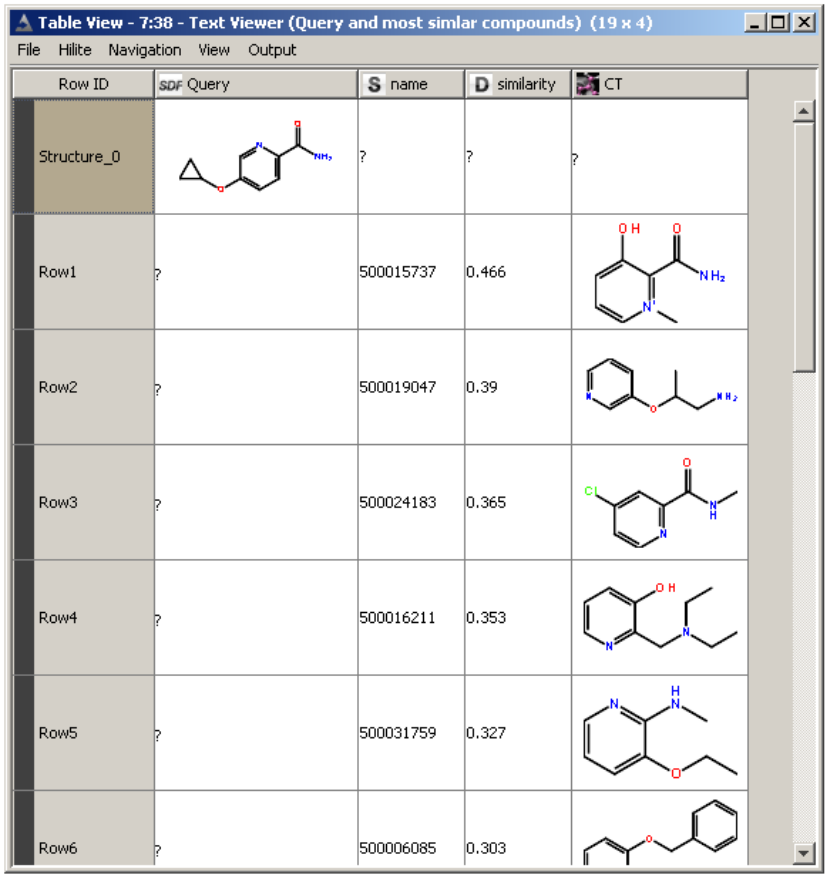
Similarity search

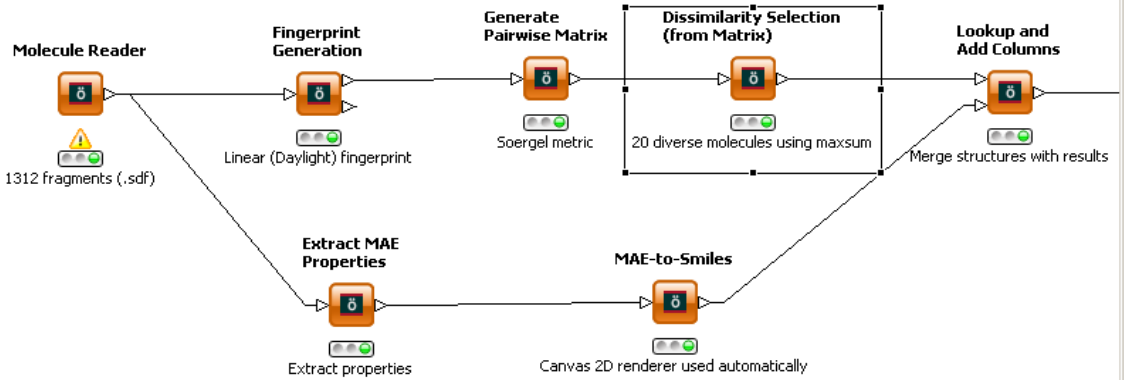


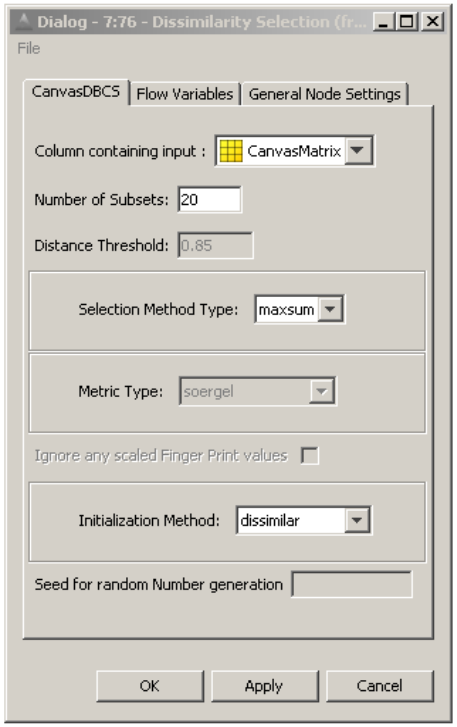


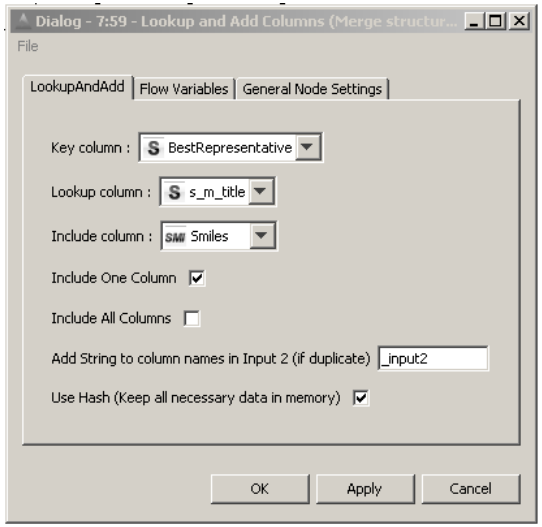


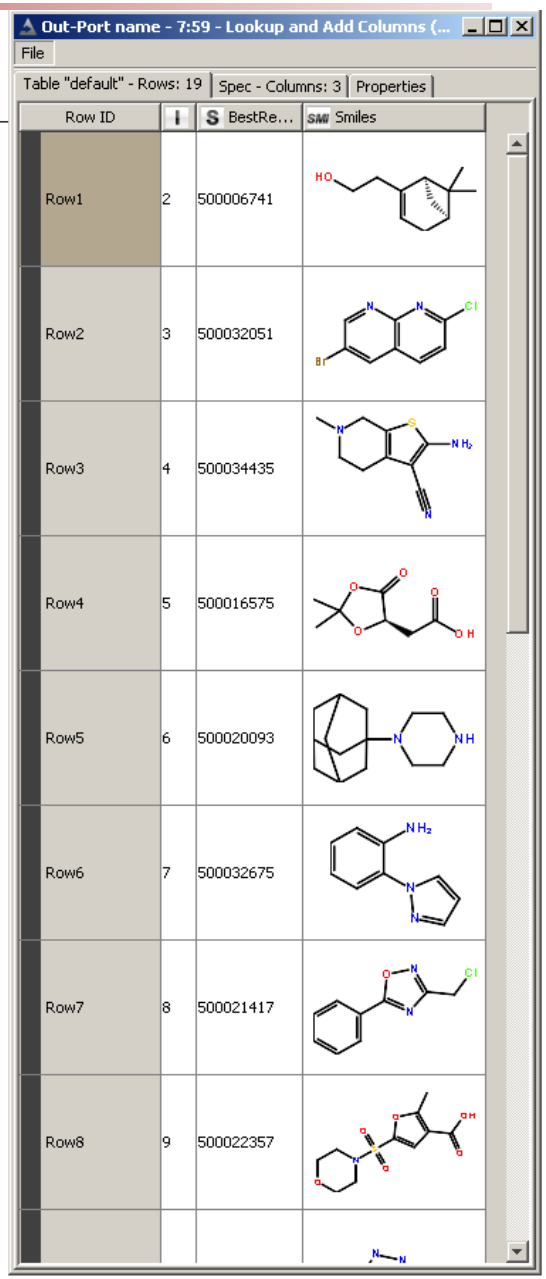
Row ID	SDF Query	S name	D similarity	CT
Structure_0		?	?	?
Row1	?	500015737	0.466	
Row2	?	500019047	0.39	
Row3	?	500024183	0.365	
Row4	?	500016211	0.353	
Row5	?	500031759	0.327	
Row6	?	500006085	0.303	

Diversity selection

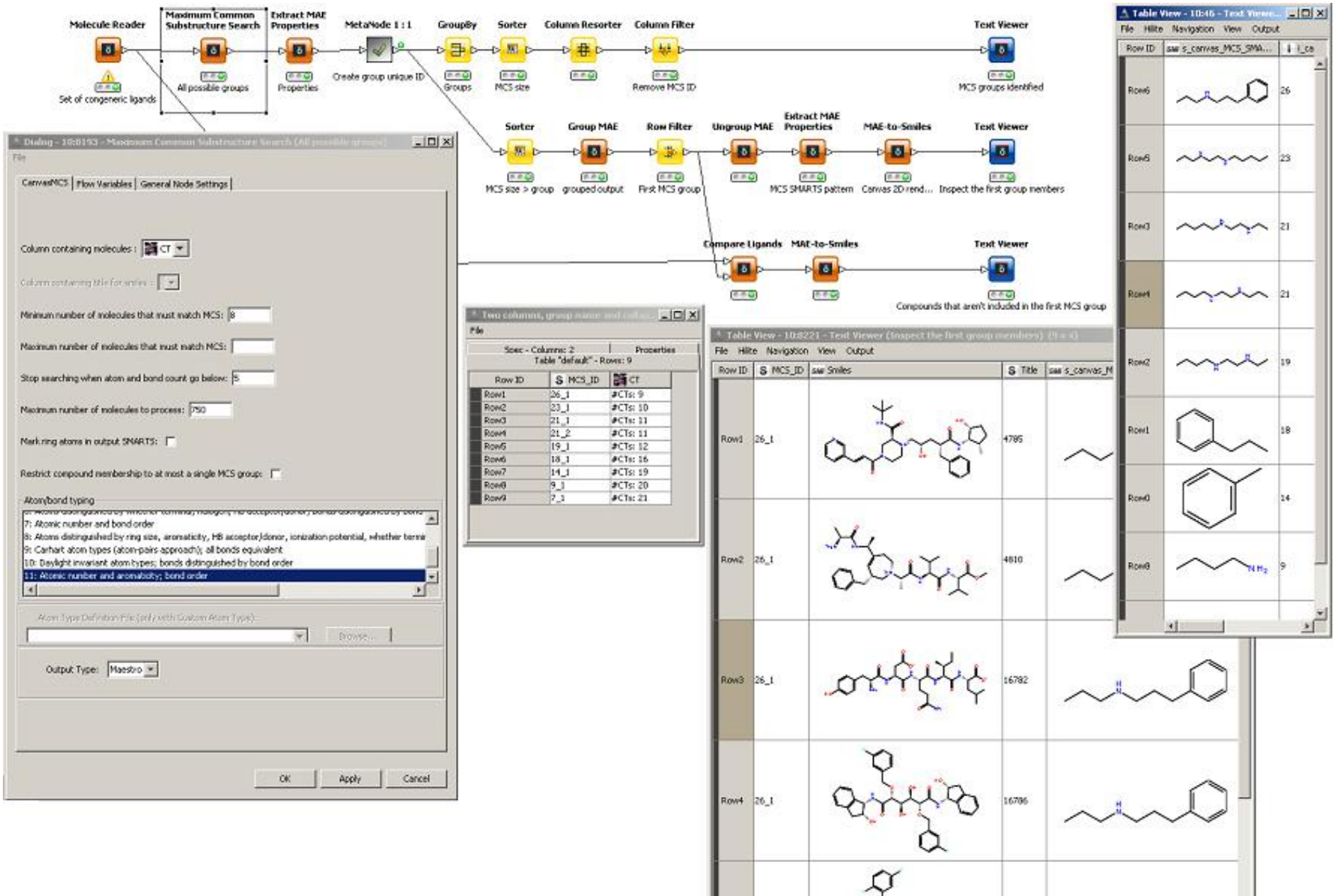




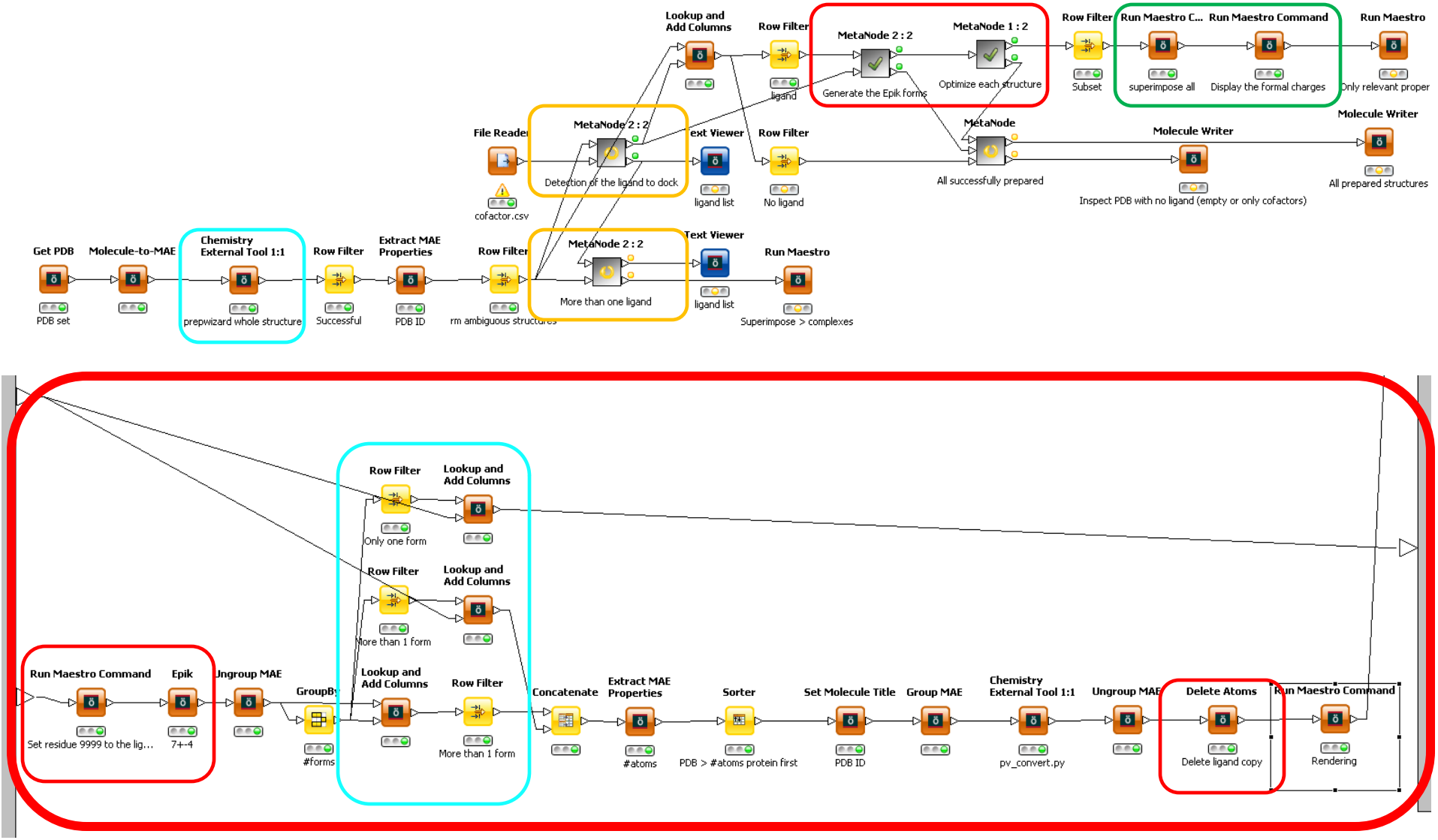




Maximum Common Substructure Search



Automatic protein preparation



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Roadmap

- Expose more back-end functionality through KNIME

  Canvas model building, Macromodel coordinate scan, CombiGlide, Desmond …
- Usability
- Stability and robustness
- Provide better integration with Maestro/Canvas
- Better integration with KNIME Enterprise products

Schrodinger KNIME extensions

Jean-Christophe **KNIME Associate Product Manager**

jcmozzic@schrodinger.com

Volker Eyrich **VP of Technology**

volker@schrodinger.com

Blaine Bell **Developer**

Hina Patel **Developer**

Schrödinger Developers

Woody Sherman **VP of Applications Science**

Applications scientists

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Why KNIME?

- Leading open-source ‘pipelining/workflow’ tool
- Extensible
- Cross-platform
- Vendor neutral
- Computational/Workflow model
- Freely available to academic and industrial researchers
- Commercial development and support
- Enterprise functionality available through KNIME.com

Timeline & Resources

- Timeline
  - Q3 2006: Started evaluation of core platform
  - Q3 2007: First release of Schrödinger extensions (version 1.0)
  - Q2 2008: Schrödinger Release 1.1 and workflow examples
  - Q2 2009: Schrödinger Release 1.2 and more examples
  - Q2 2010: New release
- Resources
  - Two 2 FTEs for development since the beginning
  - QA and documentation resources
  - Internal applications

Access to Schrödinger tools via KNIME

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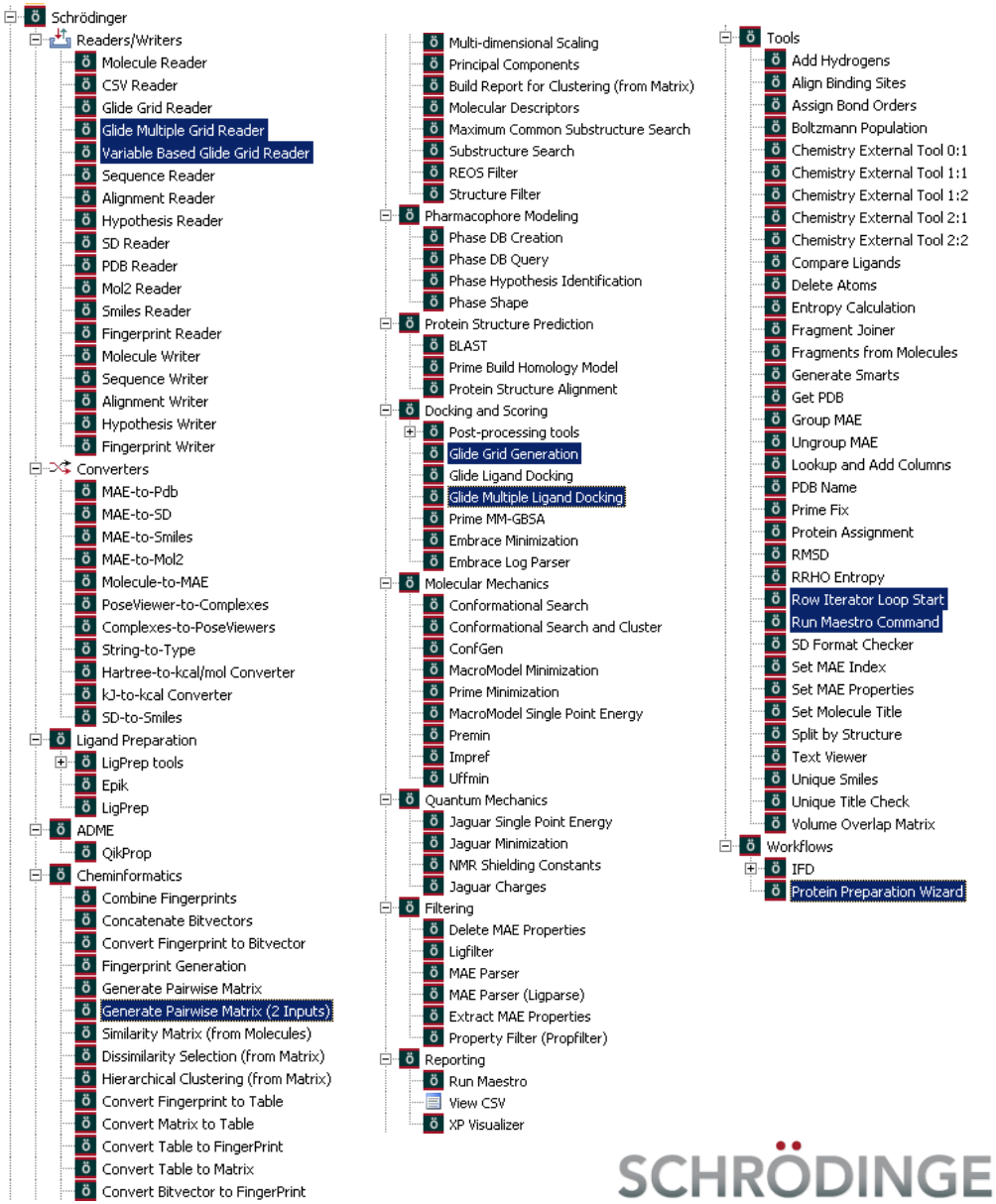
~140 nodes

- Ligand preparation
- ADME
- Cheminformatics
- Pharmacophore modeling
- Protein structure prediction
- Docking and scoring
- Molecular mechanics
- Quantum mechanics
- Workflows



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