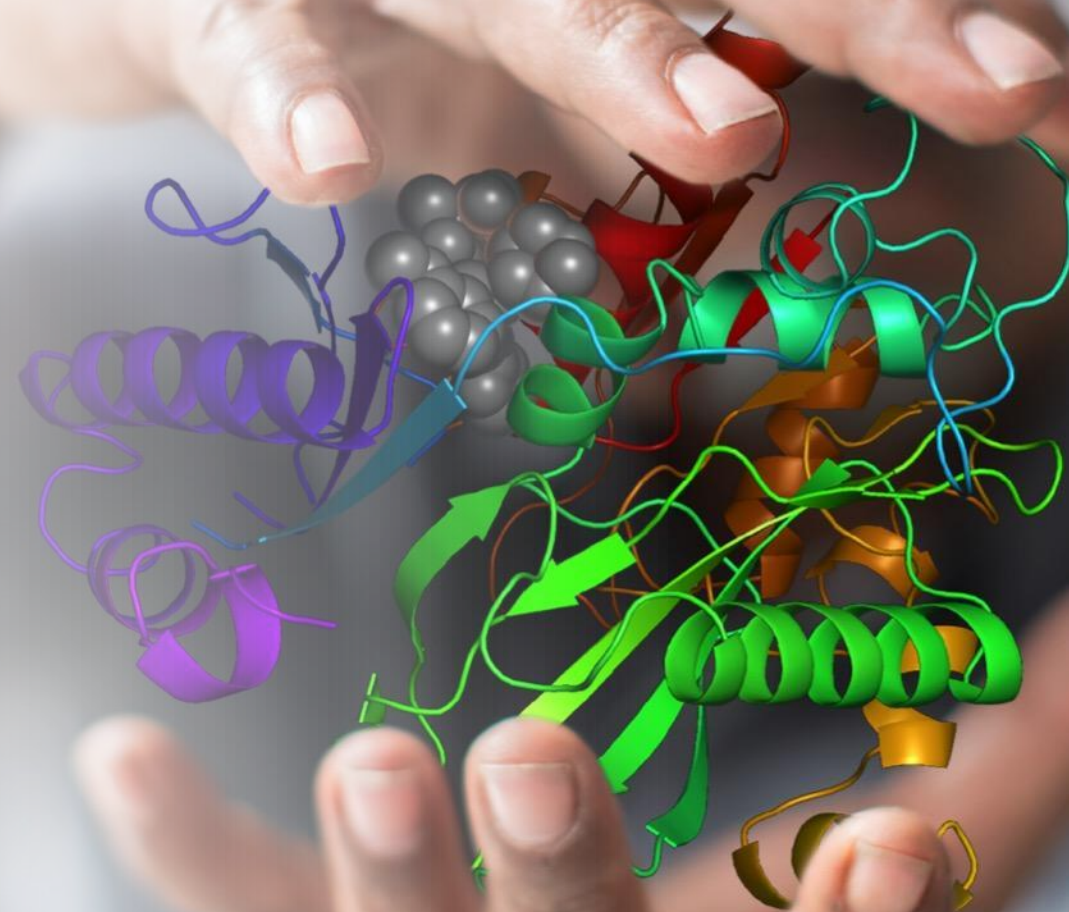


SCHRÖDINGER®

Schrödinger KNIME Extensions

New features

Jean-Christophe Mozziconacci, KNIME extension Product Manager
https://www.schrodinger.com/knimeworkflows/KNIME_newfeatures.pdf



Help and support materials

- [Product page](http://www.schrodinger.com/KNIME-Extensions) <http://www.schrodinger.com/KNIME-Extensions>
- Schrödinger Nodes on the [KNIME hub](https://hub.knime.com/schrodinger) <https://hub.knime.com/schrodinger>
- Workflow examples on the [KNIME hub](https://hub.knime.com/schrodinger) <https://hub.knime.com/schrodinger>
- Schrödinger extensions
 - Getting started manual <https://www.schrodinger.com/documentation>
 - Functionality overview http://www.schrodinger.com/upload/KNIME_Overview.pdf
 - Functionality details https://www.schrodinger.com/knimeworkflows/KNIME_newfeatures.pdf
 - FAQs <http://www.schrodinger.com/kb>
- KNIME
 - <https://www.knime.com>
 - Documentations <https://docs.knime.com>
 - All the nodes and workflow examples <https://hub.knime.com>

Installation

- The Download page:

<https://www.schrodinger.com/downloads/releases>

Update site:

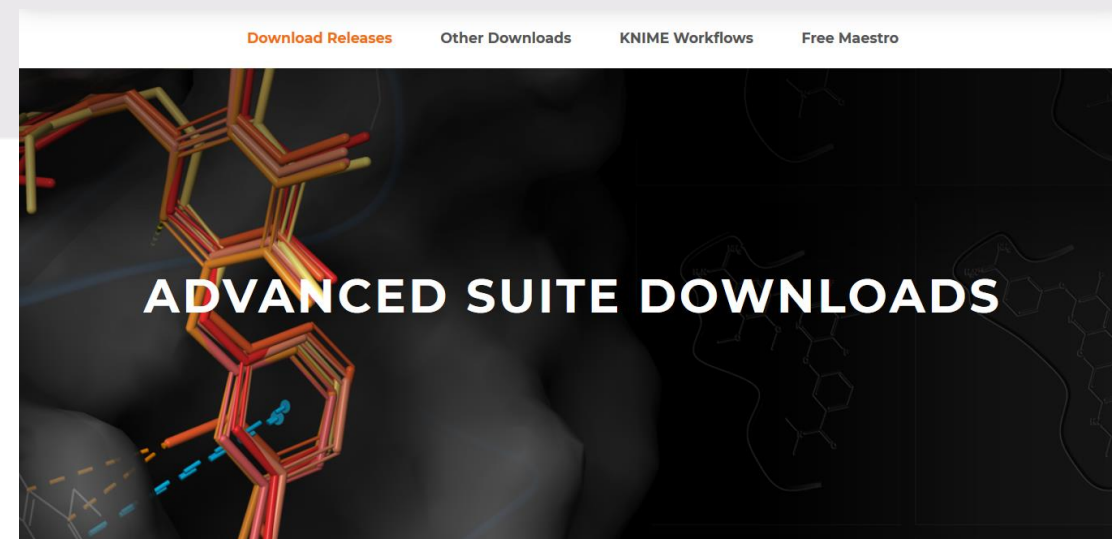
<http://content.schrodinger.com/knime/extensions> (latest)

or from the KNIME Partner Extensions:

<http://update.knime.com/partner/4.1>

<http://content.schrodinger.com/knime/previous> (previous versions)

The zipped update site is available in the installation under
\$SCHRODINGER/knime-v*/data/



Download Releases

Please choose the version of the release you'd like to download:

Version:

Release 2019-2

[VIEW LIST OF NEW FEATURES](#)

Please choose your OS:

- ☐ Linux
- ☐ Windows 64-bit
- ☐ Mac

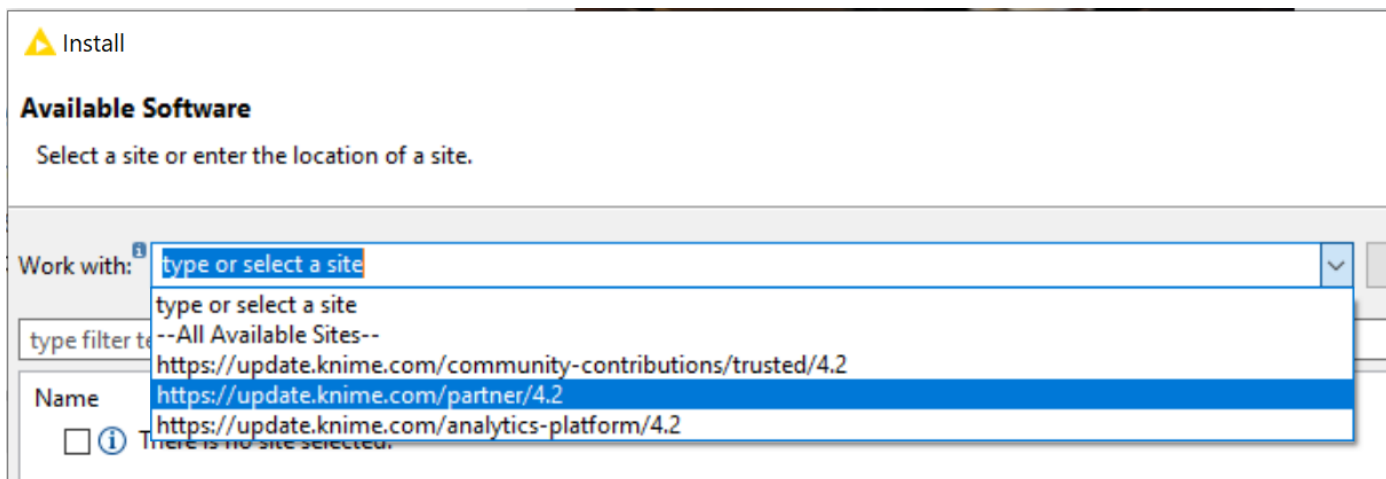
[Click here](#) to view a list of supported platforms for Release 2019-2.

Please note: Your license server software must be at least version 11.15 to be compatible with this release. See [Knowledge Base Article 338412](#) for more details.

Click here to view a list of upcoming infrastructure projects that may require changes from your IT team.

- ☒ Include KNIME Workflows (see a complete list on the [KNIME workflows](#) page)
- ☐ By downloading our software, you are agreeing to the terms set forth in our End User License Agreement (EULA), please confirm that you have read the EULA, and agree to the terms. *

[DOWNLOAD](#)



Why using KNIME

Automation

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

Collaboration

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

Prototyping

- Test parameters
- Easy result comparison and debugging
 - Data table for each step
 - e.g. Validate docking parameters

Documentation

- Various experiments and inputs
- Several branches

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

Schrödinger Nodes

160+ nodes covering the whole Schrodinger Suite

- ▼ Schrödinger
 - ▼ I/O
 - Molecule Reader (to MAE)
 - PDB Reader
 - Smiles Reader
 - Sequence Reader
 - Alignment Reader
 - Canvas Fingerprint Reader
 - QSAR Model Reader
 - Phase Hypothesis Reader
 - Glide Grid Reader
 - Desmond CMS Reader
 - Desmond Trajectory Reader
 - FEP+ Reader
 - Molecule Writer (from MAE)
 - Sequence Writer
 - Alignment Writer
 - Phase Hypothesis Writer
 - Glide Grid Writer
 - Canvas Fingerprint Writer
 - QSAR Model Writer
 - ▼ Converters
 - Molecule-to-MAE
 - MAE-to-Pdb
 - MAE-to-SD
 - MAE-to-Smiles
 - MAE-to-Mol2
 - SD-to-Smiles
 - PoseViewer-to-Complexes
 - Complexes-to-PoseViewers
 - String-to-Type
 - Hartree-to-kcal/mol Converter
 - kJ-to-kcal Converter
 - ▼ Ligand Preparation
 - LigPrep Steps
 - Epik
 - LigPrep
 - ▼ ADME and Molecular Properties
 - QikProp
 - Canvas Molecular Descriptors
 - Maestro Molecular Properties
 - ▼ Pharmacophore Modeling
 - Shape Screening
 - Phase Screening
 - Phase DB Creation
 - ▼ Library Enumeration
 - ▼ Fragments
 - Fragment Joiner
 - Fragments from Molecules
 - Bioisostere Replacement
 - Reaction Based Enumeration
 - ▼ Protein Preparation and Refinement
 - Prime Macrocyclic Sampling
 - Protein Preparation Wizard
 - Protein Assignment
 - BLAST
 - Prime Build Homology Model
 - Prime Minimization
 - Prime Energy
 - Prime Refine Loops
 - Prime Side Chain Sampling
 - Residue Scanning
 - Induced Fit Docking
- ▼ Cheminformatics
 - ▼ Fingerprint Based Tools
 - Canvas Fingerprint Generation
 - Generate Pairwise Matrix
 - Generate Pairwise Matrix (2 Inputs)
 - Similarity Matrix (from Molecules)
 - Dissimilarity Selection (from Matrix)
 - Hierarchical Clustering Report
 - Hierarchical Clustering
 - ▼ Filters and Mining Tools
 - Substructure Search
 - Maximum Common Substructure Search
 - REOS Filter
 - Structure Filter
 - ▼ Utilities and Converters
 - Principal Components
 - Multi-dimensional Scaling
 - Combine Canvas 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
 - Bayes Classification Prediction
 - PLS Model Building
 - PLS Prediction
 - AutoQSAR Build Model
 - AutoQSAR Predict

Schrödinger Nodes

- ▼  Docking and Scoring
 - ▼  Post-processing
 -  Prime MM-GBSA
 -  Embrace Minimization
 -  Strain Rescore
 -  Pose Entropy
 -  Pose Filter
 -  Glide Ensemble Merge
 -  Glide Merge
 -  Glide Sort Results
 -  Glide Grid Generation
 -  Glide Ligand Docking
 -  Glide XP Visualizer
 -  Covalent Docking
- ▼  Molecular Mechanics
 - >  Minimization
 - ▼  Conformational Search
 -  MacroModel Coordinate Scan
 -  MacroModel Conformational Search
 -  ConfGen
 -  MacroModel Single Point Energy
 -  Conformer Cluster
 - ▼  Molecular Dynamics
 -  Desmond System Builder
 -  Desmond Molecular Dynamics
 -  Desmond Trajectory Extract Frames
 -  Desmond Trajectory Manipulation
 - ▼  Quantum Mechanics
 -  Conformer and Tautomer Predictor
 -  Jaguar Single Point Energy
 -  Jaguar Minimization
 -  Jaguar NMR Shielding Constants
 -  Jaguar Charges
 -  Semiempirical NDDO
 - ▼  General Modeling
 -  Ligfilter
 -  Property Filter (Propfilter)
 -  SiteMap
- ▼  Reporting
 -  Run Maestro
 -  KNIME-Maestro Connector
 -  Run PyMOL
 -  Run Spreadsheet Viewer
 -  Table Viewer
 -  Multiple Sequence Viewer
 - ▼  LiveDesign
 -  Import from LiveDesign
 -  Export to LiveDesign
 -  Export images to LiveDesign
 -  Upload model to LiveDesign
 -  Upload Server to LiveDesign
 - ▼  Scripting
 -  Run Maestro Command
 -  Chemistry External Tool
 -  Python Script 0:1
 -  Python Script 1:0
 -  Python Script 1:1
 -  Python Script 1:2
 -  Python Script 2:1
 -  Python Script 2:2
- ▼  Miscellaneous
 - ▼  Data Manipulation
 -  Compare Ligand Sets
 -  Lookup and Add Columns
 -  Group MAE
 -  Ungroup MAE
 - ▼  Structure Manipulation
 -  Add Hydrogens
 -  Delete Atoms
 -  Split by Structure
 -  Extract Atom/bond Properties
 - ▼  MAE Property Manipulation
 -  Extract Properties
 -  Set MAE Properties
 -  Set Molecule Title
 -  Set MAE Index
 -  Unique Title Check
 -  Delete MAE Properties
 - ▼  Utilities
 - >  Protein
 -  RMSD
 -  Generate Unique Smiles
 -  Generate Smarts
 -  Entropy Calculation
 -  Volume Overlap Matrix
 -  Boltzmann Population
 -  SD Format Checker
 -  Set PDB Name
- ▼  Tools
 -  Job Control
 -  Postmortem
 -  Setup Diagnosis
 -  Workflow List
 -  Get Help
 -  Batch Test


















































KNIME Workflow Page – Workflow Examples

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

or https://hub.knime.com/schroedinger/spaces/Workflow_examples/latest/










- ▼ _Nodes
 - > Conformer cluster
 - > Epik
 - > Free nodes
 - > Multiple Sequence Viewer
 - > Readers and Writers
 - > Run Maestro
 - > Tools
 - > Workbench- most commonly used nodes
- ▼ Cheminformatics
 - > AutoQSAR
 - > Clustering
 - > Database analysis
 - > Diversity
 - > MCSS
 - > Similarity
 - > Substructure
- ▼ Docking
 - > Binding site
 - > Covalent docking
 - > Docking
 - > Ensemble docking
 - > Grid generation
 - > Loop over parameters
 - > Validate parameters
 - > Virtual screening
- ▼ General
 - > Output column structure
 - > P450 Site of Metabolism
 - > Unique molecule titles
- ▼ Labs
 - > Parameter flow variables
- ▼ Library design
 - > Bioisoster replacement
 - > Enumeration
 - > Library design workshop
 - > Reaction-based enumeration
- ▼ LiveDesign
 - > Import and export
 - > Related PDB structures
 - > Upload as Computational model
 - > Upload from KNIME server
- ▼ Molecular Dynamics
 - > Binding Pose Metadynamics
 - > FEP
 - > Ligand alignment MD refinement
 - > MD simulation
- ▼ Molecular Mechanics
 - > Compare confo search methods
 - > Conformational search

KNIME Workflow Page – Workflow Examples

- ▼  Pharmacophore
 - >  Phase screening
 - >  Shape screening
- ▼  Protein
 - >  Alignment
 - >  Bioluminate
 - >  Build antibody
 - >  Induced-fit docking
 - >  Missing loop refinement
 - >  Model building
 - >  Reactive protein residues
 - >  Sequence Converter
 - >  Split and align multimers
 - >  Watermap
- ▼  Quantum Mechanics
 - >  Conformational search
 - >  Conformer et tautomer prediction
 - >  ESP charges
 - >  Jaguar pKa
 - >  QM descriptors
 - >  QM properties
 - >  Semiempirical NDDO
- ▼  Real world
 - >  Binding site shape clustering
 - >  Cocrystallized ligand redocking
 - >  Database preparation
 - >  Protein model building
 - >  Protein structural diversity analysis
 - >  Sitemap and docking
- ▼  Scripting
 - >  Chemistry external tool
 - >  Maestro commands
 - >  Python script
- ▼  Server
 - >  AutoQSAR
 - >  Setup diagnosis
- ▼  Tools
 - >  Batch execution
 - >  Installation
 - >  Jobcontrol
 - >  Workflows list
- ▼  Visualization
 - >  KNIME-Maestro connector
 - >  Run Maestro
 - >  Run PyMOL
- ▼  Workbench
 - >  Group looper
 - >  GroupBy
 - >  Unpivot

KNIME Live-Design models

https://hub.knime.com/schroedinger/spaces/LiveDesign_models/latest/

- ▼  ADME and molecular properties
 - ▲ ADME
 - ▲ Atropisomerism
 - ▲ ESP surface
- ▼  Docking
 - ▲ Docking and protein surface
 - ▲ Docking and rendering
 - ▲ Ensemble docking
- ▼  Ligand preparation and library design
 - ▲ Bioisosteres
 - ▲ Low energy conformation
 - ▲ Protonation forms
- ▼  Miscellaneous
 - ▲ Basic example
 - ▲ FEP analysis
 - ▲ Installation test
- ▼  Plotting
 - ▲ Ligand CNS desirability plot
 - ▲ Ligand CNS desirability range plot
 - ▲ Ligand property radar plot
- ▼  Protein preparation and refinement
 - ▲ Cocrystallized ligands
 - ▲ Get PDB
- ▼  QSAR
 - ▲ Random forest
- ▼  Run on a KNIME Server
 - ▲ My workflow running on a KNIME server
- ▼  Structure alignment
 - ▲ Ligand alignment
 - ▲ Pharmacophore screening

New features in the KNIME extension

In Schrödinger Suite 2023-4

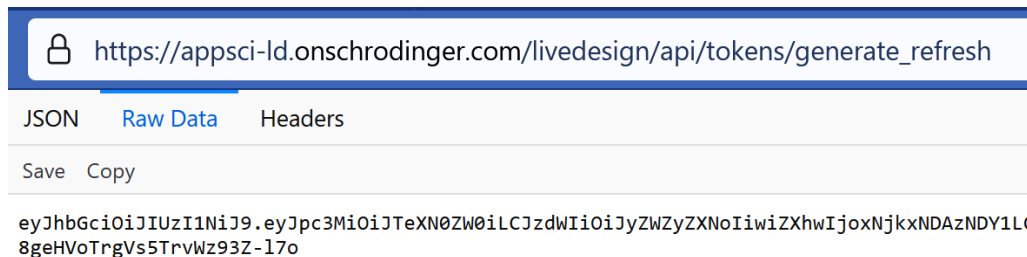


2023-4 New Features

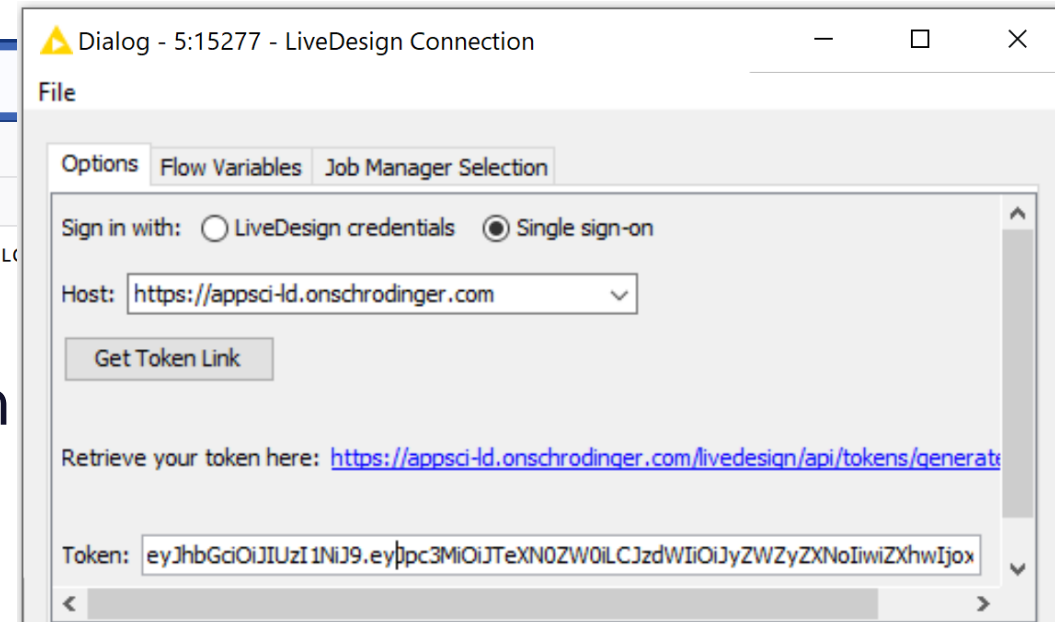
- The LiveDesign connection node supports Single Sign-On and reconnection to hosts running different LiveDesign versions
It can be connected to the Upload as LiveDesign node
- LiveDesign settings are stored as profiles in the preferences panel for multiple hosts
- Images can be exported to a LiveReport including generic entities

LiveDesign connection – Single Sign-On

- The LiveDesign connection node can use Single Sign-On (SSO) tokens
 - It streamlines the login process and exchanging workflows with colleagues
 - The SSO tokens are saved in the KNIME preferences (ie workspace) for each host across KNIME sessions
 - But not saved in the node configuration for security reason
 - When a workflow is shared with colleague, his/her SSO will be used
 - No need to change the username and password each time
 - SSO loaded in new node in the workflow after selecting the host

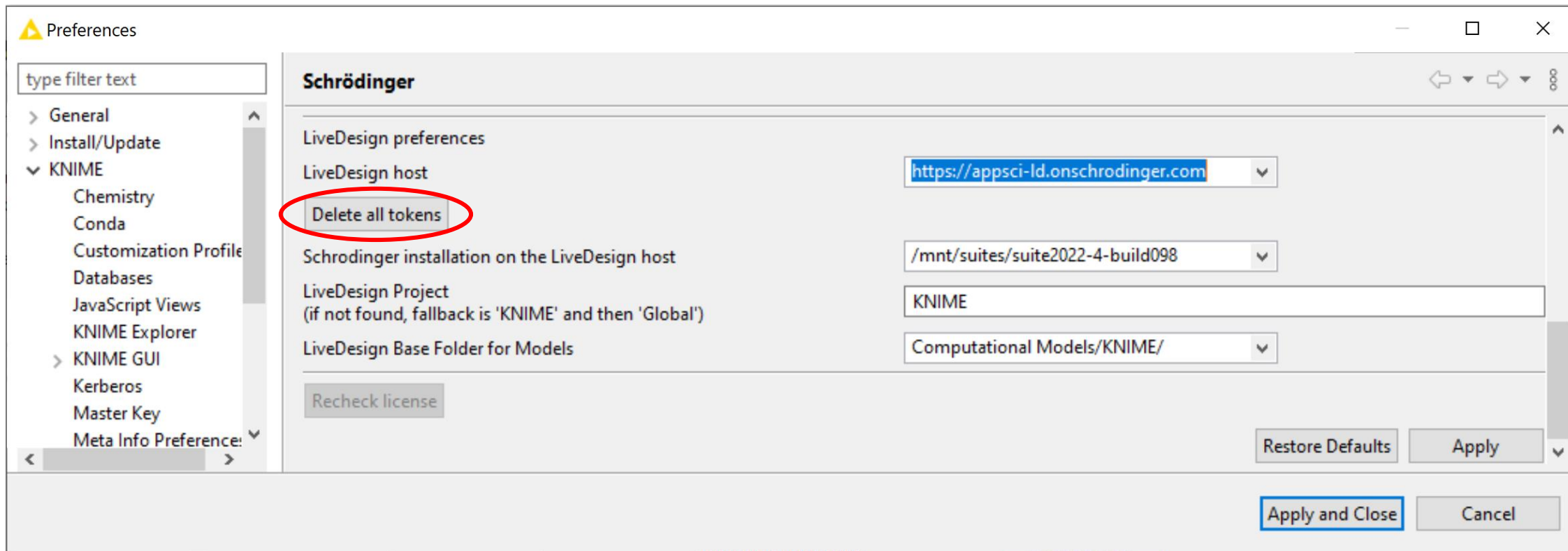


- Reconnect to hosts with any LiveDesign version
 - No need to restart KNIME (same as in Maestro)



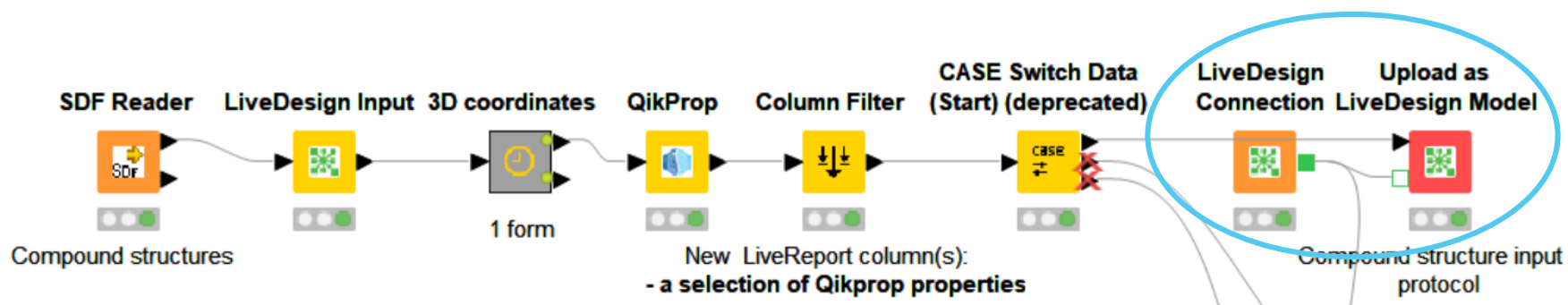
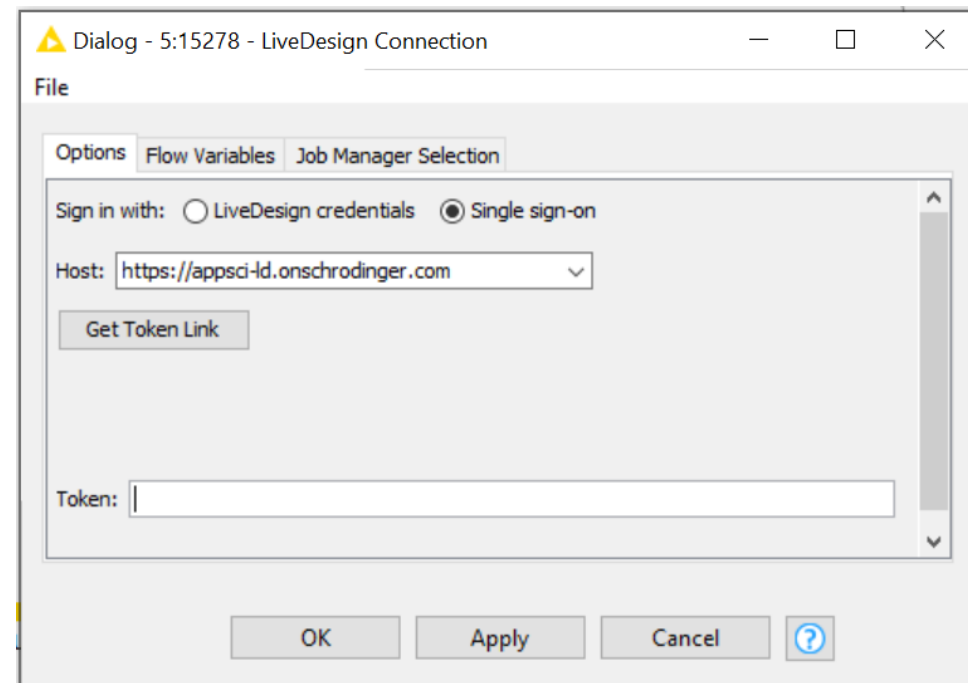
LiveDesign connection – clear SSO tokens

- Delete SSO tokens
 - Equivalent to “disconnect” in Maestro
 - For a specific host: In the Connection node, empty the SSO field and click Apply
 - Delete all tokens button in KNIME preferences



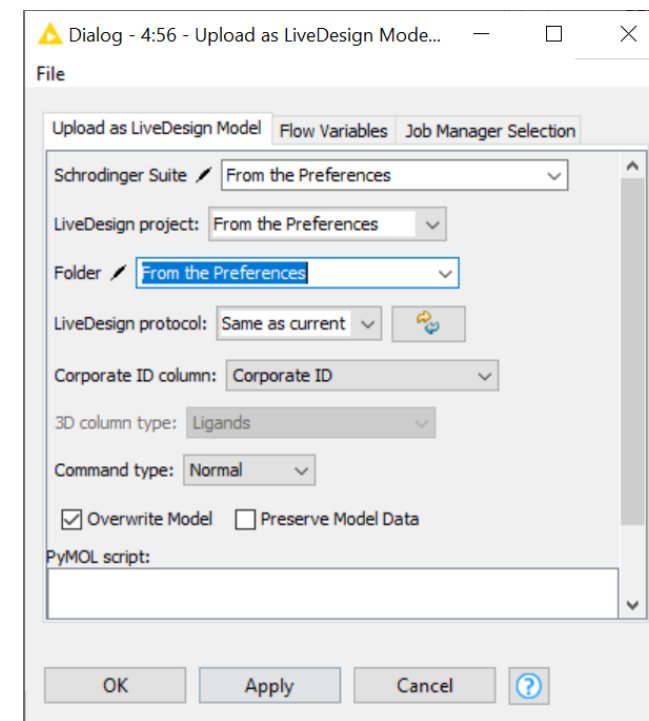
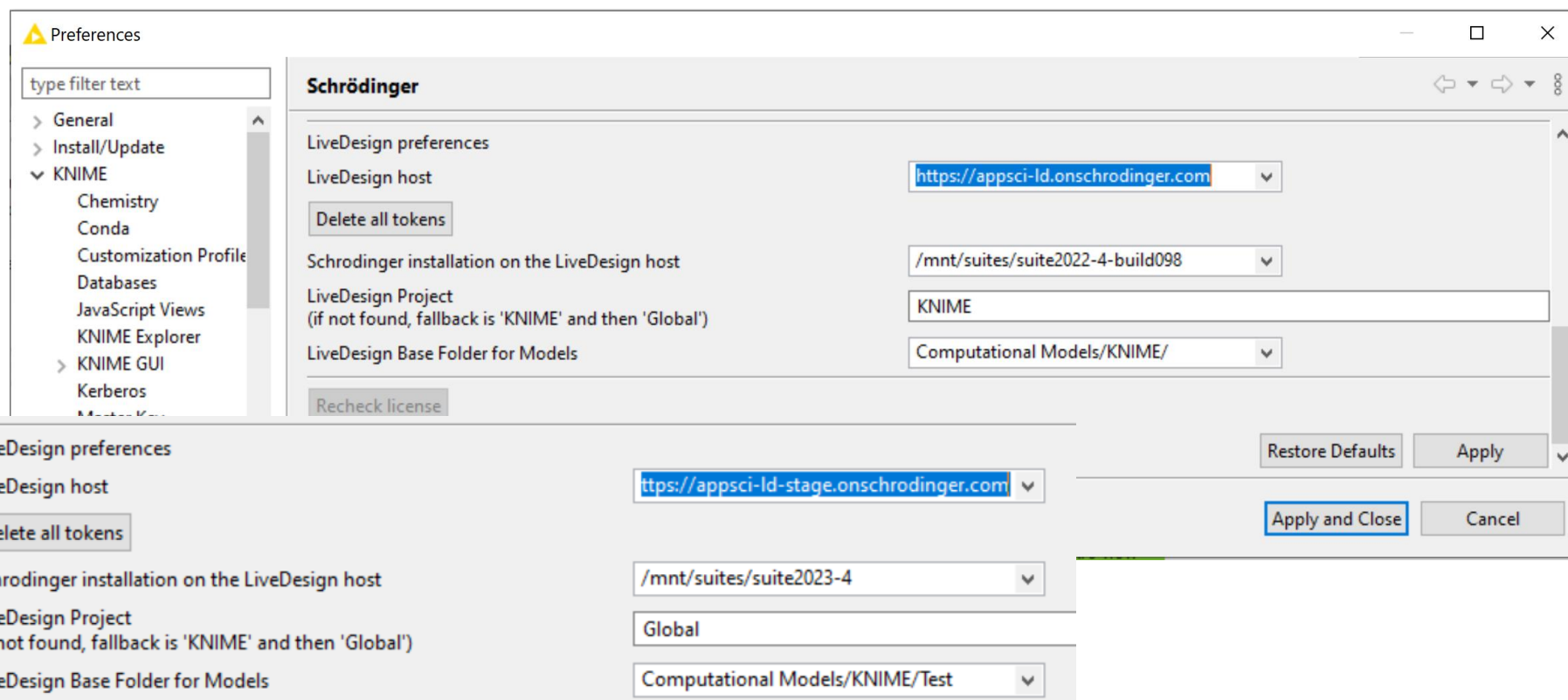
LiveDesign connection to Upload as model node

- Standardized with most import LiveDesign nodes (import and export nodes)
 - Takes advantage of the SSO, profile
 - eg when exchanging workflows with colleagues
- The Credential configuration node is still supported in old workflows
- Reduced the configuration panel opening time
 - The project and protocol lists are populated on demand



LiveDesign setting profile

- A profile is saved for each host in the Preferences panel
 - Saves setting sets for the Upload as LiveDesign model node
 - eg typical application: switch easily between a production and a testing LiveDesign machine
- The values are updated in the panel when the LiveDesign host field is changed
 - Edited fields can be saved by clicking on the Apply button

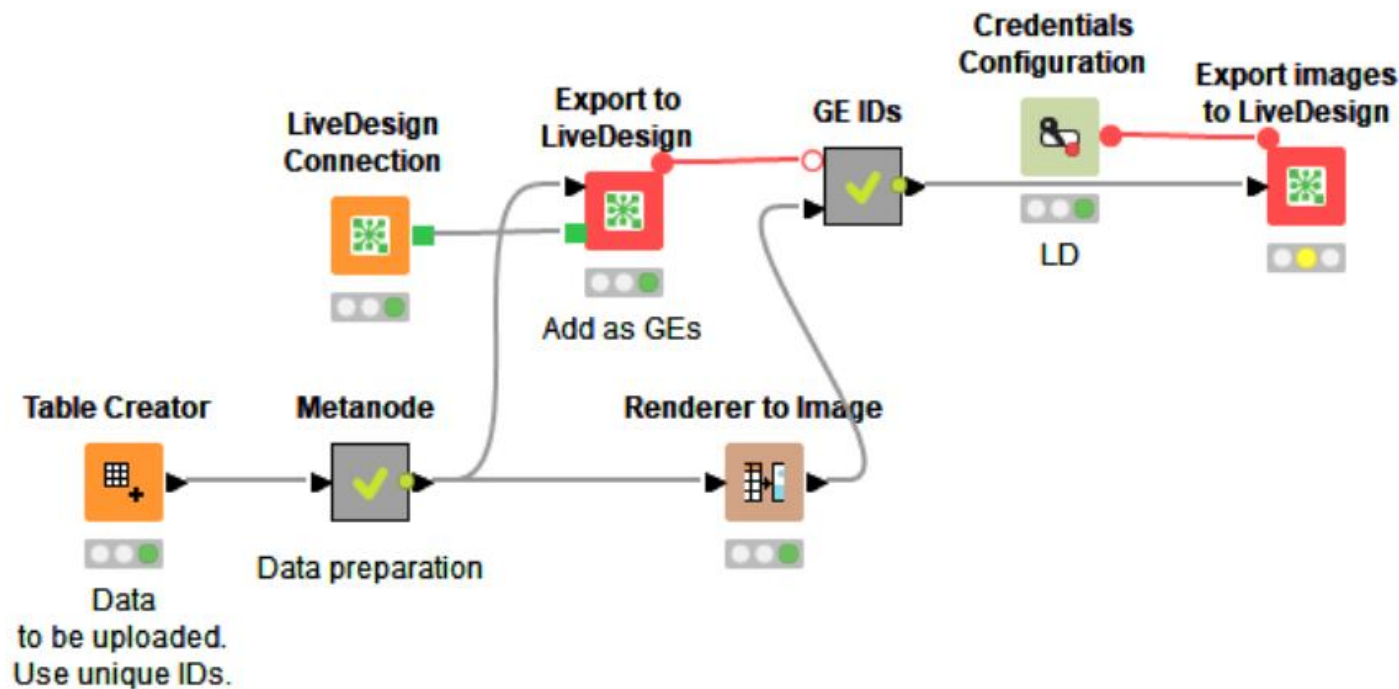


Using a production and testing LiveDesign machine

- With the improvements to streamline the integration of KNIME sessions and LiveDesign servers
 - More user friendly
 - Save time
 - Less error prone
- Switch between production and test machines
 - Set the host in the LD connection node
 - No reconfiguration required for usual scenarios:
 - The SSO is saved
 - The settings are taken from the profile in KNIME preferences
 - No need to restart KNIME even if the LiveDesign versions differ

Miscellaneous

- Export images to a LiveReport including Generic entities
 - The ID mapping is stored in a temporary file
 - The filepath is in ge_id_mapfile flow variable. See the corresponding workflow example.



2023-3 New Features

- Support for KNIME v5.1 added

In LiveDesign nodes:

- The Livedesign connection node can use Single Sign-On (SSO) tokens to streamline the login process

New features in the KNIME extension

In Schrödinger Suite 2023-2



2023-2 New Features

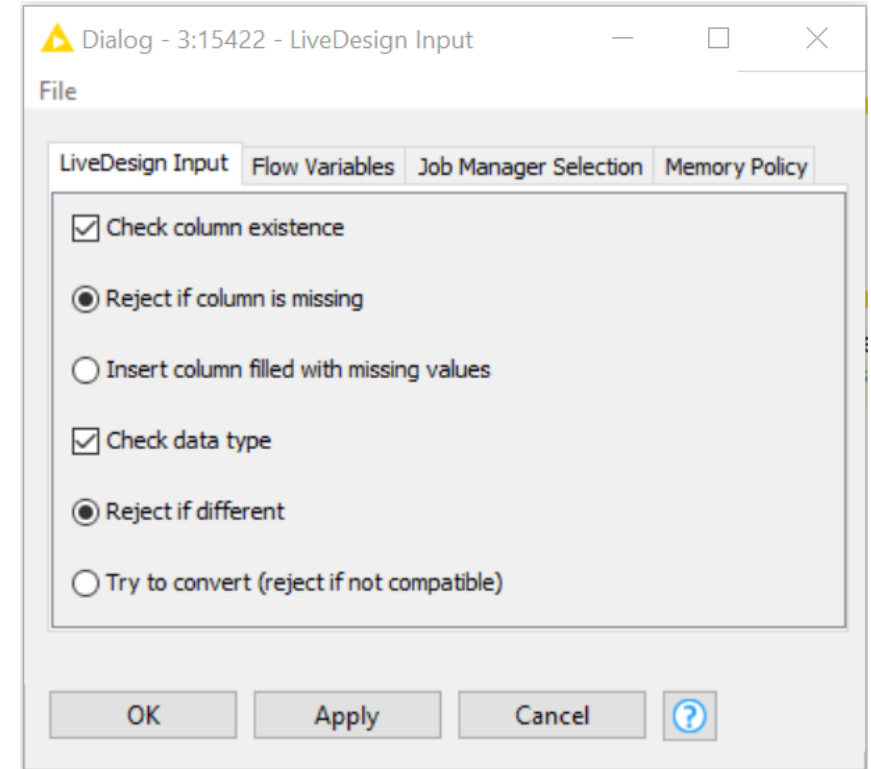
- Includes the latest version of KNIME (v4.7)
- Improved usability of the Extract Properties node configuration panel

In LiveDesign nodes and protocols:

- - Adaptable input column checking of the LiveDesign input node
- - KNIME protocol section to install extra KNIME extensions is more robust

LiveDesign input node column input checking

- For parametrized models, a clear error message is printed in on the Tasks page if the input column checking detects discrepancies between the user column selection from the current LiveReport and the data used to create the workflow
 - It makes easy for the user to realize inappropriate column or selection mistake
- The column checking can be adapted to the downstream workflow which can be more or less tolerant to variabilities eg:
 - Integer/double numbers
 - String / numbers
 - Missing columns
- Also numeric corporate IDs are now supported by this node



New features in the KNIME extension

In Schrödinger Suite 2023-1



2023-1 New Features

- Support for KNIME (v4.7) added
- Enhanced robustness of the Extract Properties node where new properties can now be included or excluded
- The LigPrep node reads setting files exported from Maestro
- The new protein preparation workflow node configuration panel is identical to Maestro's

Improvements to LiveDesign Import and Export nodes:

- Export structures to LiveDesign as generic entities
- Move beyond ligands and proteins to import any 2D/3D structure into LiveDesign as generic entities
- The LiveDesign connection node takes the host from KNIME preferences

KNIME 4.7 – Python integration and some new features

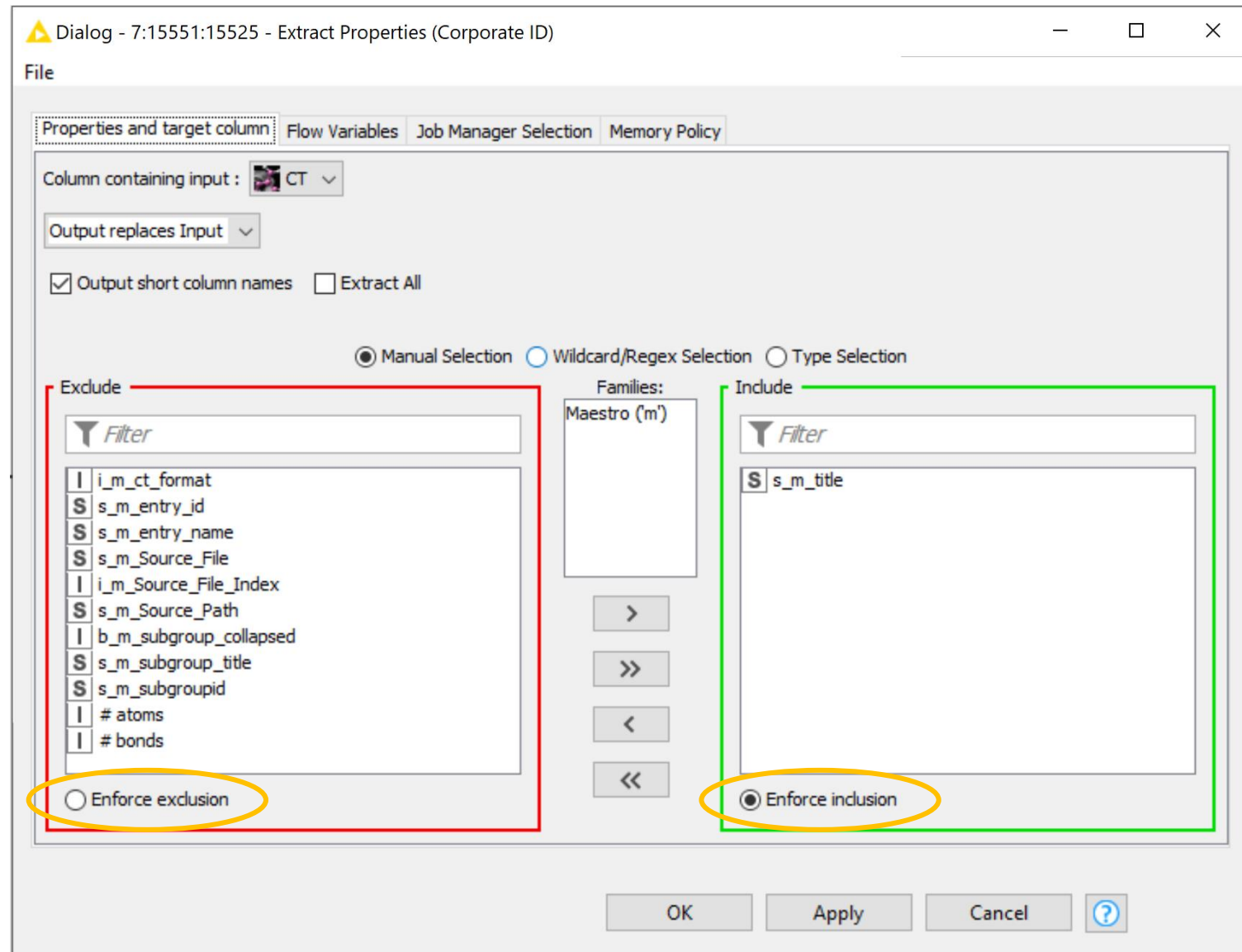
- Modern UI/UX
- New Visualization Nodes
 - box plot, density plot, heatmap, histogram, pie chart, stacked area chart, and statistics
- Geospatial Analysis
- Improved Integration Between KNIME and Python
 - Much faster data transfers between KNIME and Python
 - A better Python API (especially for chemical types)
 - A bundled Python environment
- New Python View Node
 - Supporting HTML based views which allow for interactive plots
- Enhancements to KNIME Python Extension Development (Labs)
- More Efficient Connectivity/File Handling
 - New DB Row Manipulator node and other node improvements
- Connecting Multiple Workflows
 - Independent of Workflow Location
 - Container Input (Raw HTTP) and Container Output (Raw HTTP) have been added to define generic REST APIs via KNIME workflows
- New functionalities
 - Row To Column Header is a new node to extract a data row and convert it into the column header.
 - The Sorter and Top K Selector nodes can sort strings alphanumerically
- Native KNIME Builds for Apple Silicon Processors

The compatible version is available on the Partner update site: <https://update.knime.com/partner/4.7>

See details in <https://www.knime.com/whats-new-in-knime-analytics-platform-47>

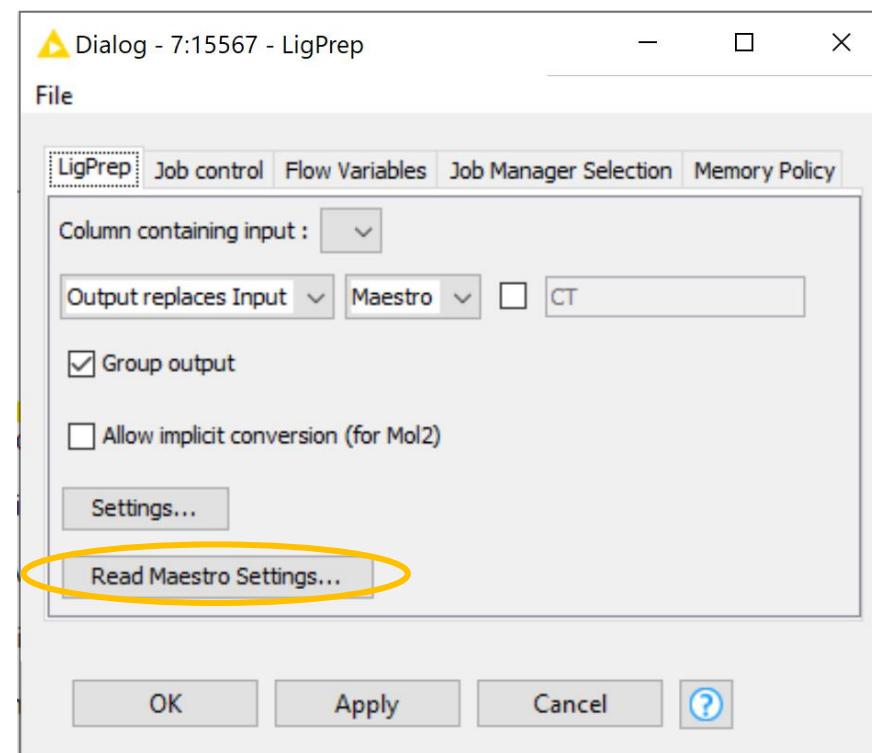
Extract properties – include or exclude the new properties

- Enforce exclusion or inclusion
 - Of the new properties
 - Standard KNIME filtering components
- More robust property list update when the upstream workflow is edited



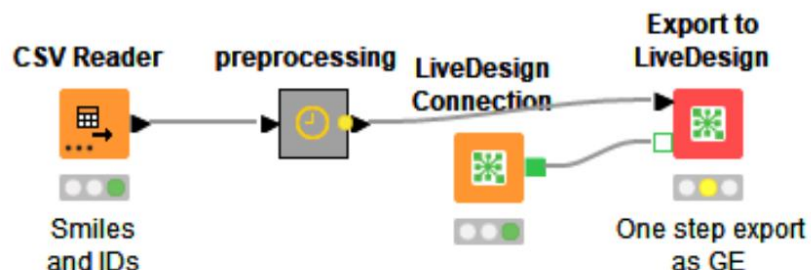
Other node improvements

- Protein preparation workflow node
 - Uses the same configuration panel as Maestro
 - The new node is feature complete
 - The old node is retired but it can still run in existing workflows
- The LigPrep node reads setting files exported from Maestro
 - To replicate easily Maestro or LiveDesign calculations
 - Same functionality already available in Glide docking node

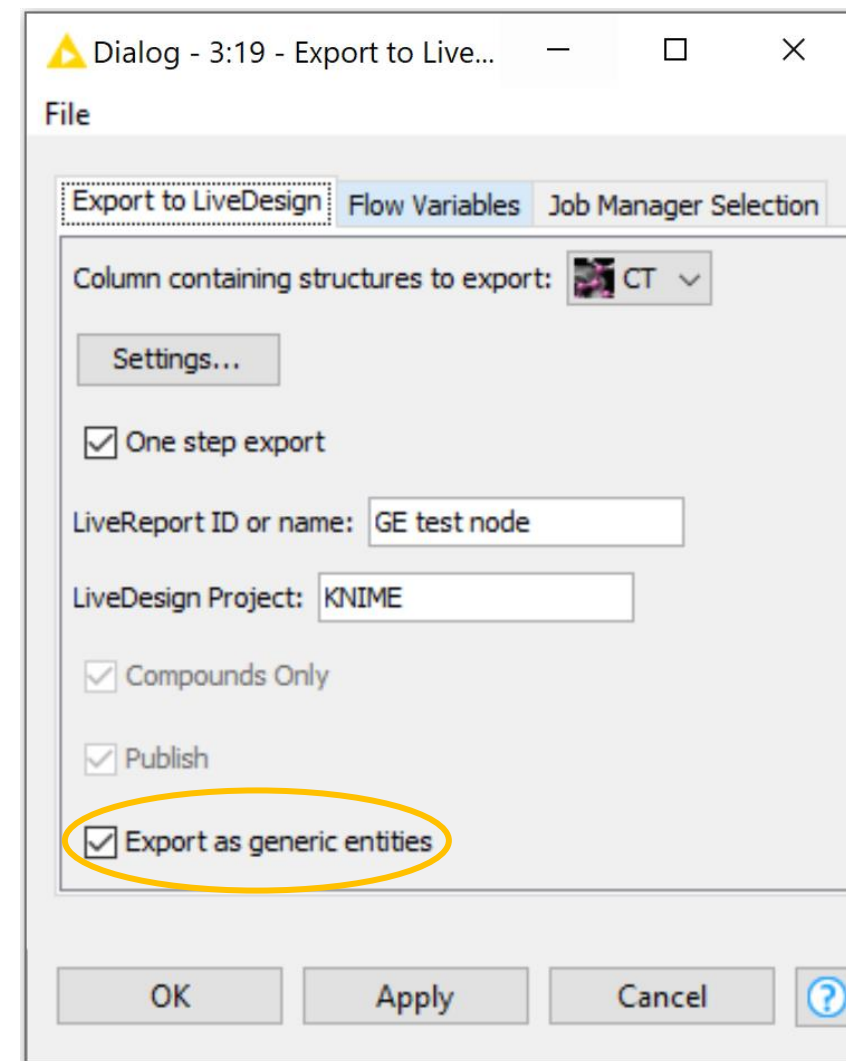


Export to LiveDesign – as generic entities

- In the One step export mode
 - Deduplication based on the provided corporate ID
 - ID from the Maestro or sdf structure title
 - or the first column after the smiles column in the input table
 - Upload scenarios:
 - Several entities can have the same structure (same smiles/maestro file with different specified IDs)
 - eg Material Science applications
 - Several structures per Corporate ID

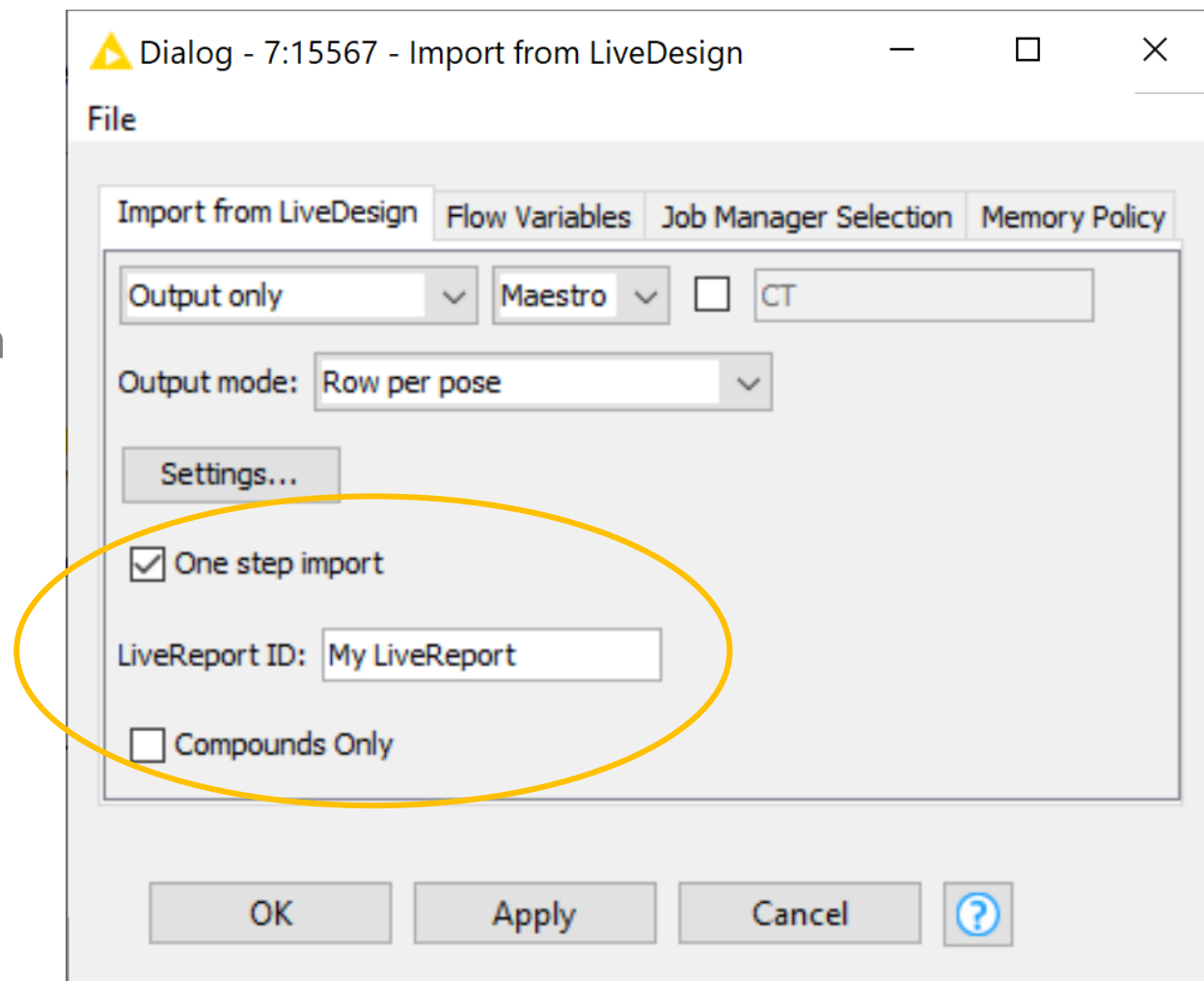


In LiveDesign version older than 22-3, a loop is required as only 1 Generic Entity can be exported at a time



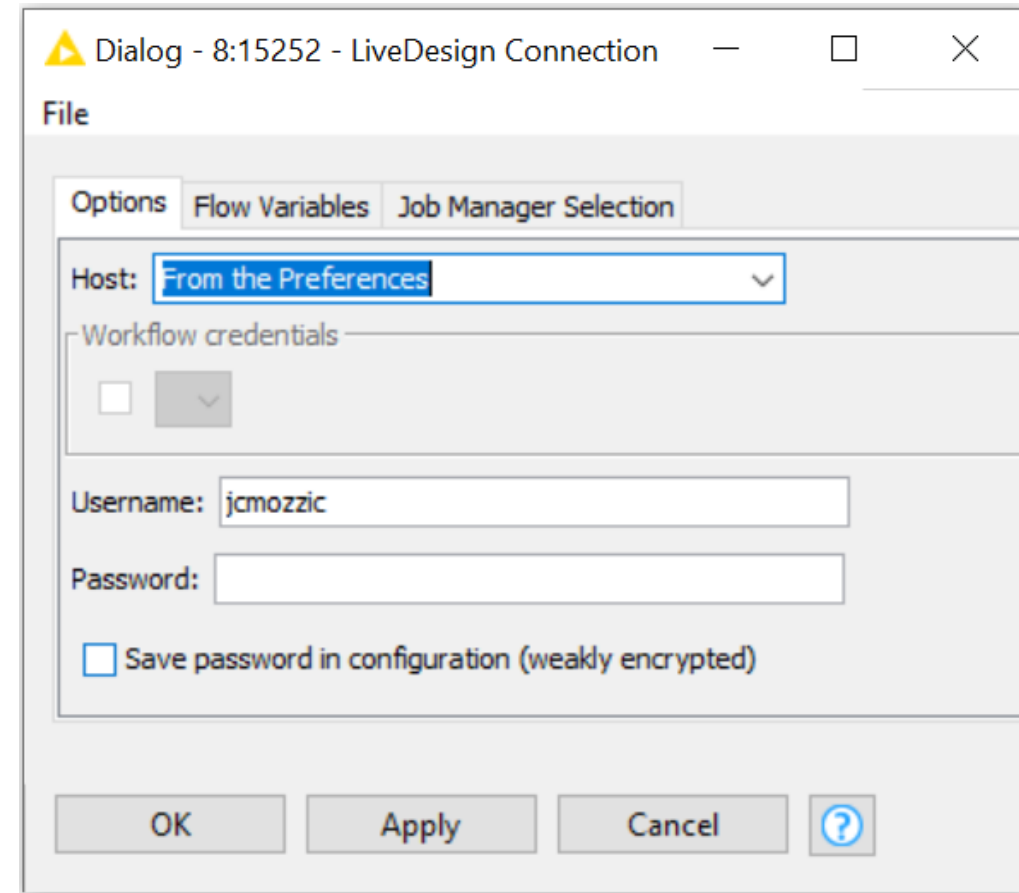
Import from LiveDesign – the whole LiveReport

- No configuration needed
- Relevant columns filtered downstream
- Similar mode already available in the Export to LiveDesign node
- Use cases:
 - Import columns with the same name from different LiveReports
 - Column of interest or column names change
 - In workflows to be run on the KNIME server



Other KNIME in LiveDesign improvements

- LiveDesign connection node takes the host from KNIME preferences
 - Same as the Upload as LiveDesign model node
- Don't save the executed workflow when running a KNIME protocols
 - With the -no_knwf option the executed workflow file won't be saved
 - eg when the workflow is too large for the disk space
 - By default it is stored with the output files. So the model doesn't have to be run again to investigate unexpected results.



New features in the KNIME extension

In Schrödinger Suite 2022-4



2022-4 New features

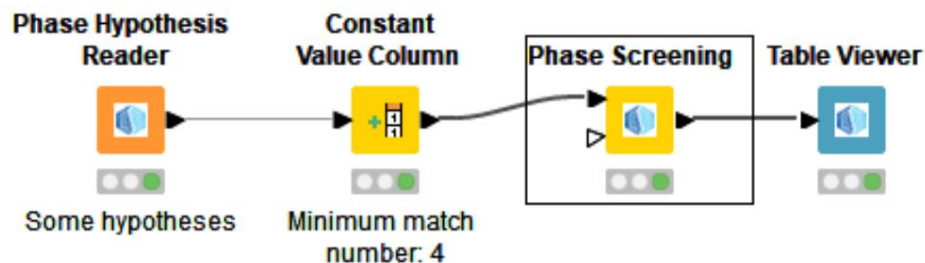
- Includes the latest version of KNIME (v4.6.1)
- The number of matches can be controlled in the Phase screening node
- SiteMap and QSAR Predict nodes are more robust
- KNIME from Maestro is planned to be retired

In LiveDesign:

- When deploying a model the suitable KNIME protocol is chosen automatically and the latest version of the protocol uploaded
- Distribution of calculations is controlled from the model admin page
- Model changes from LiveDesign Admin page can be preserved when overwriting an existing model
- A new administration node to move, archive and unarchive models

Phase screening node and KNIME from Maestro

- Phase screening node
 - The number of matches can be controlled from input table columns and set for each hypothesis



Output table - 3:8332 - Constant Value Column (Minimum match number: 4)

| Row ID | Hypothesis | Minimum match number |
|--------|-------------------------------------|----------------------|
| Row0 | Hypothesis:AADPR_75 Size=7350 by... | 4 |
| Row1 | Hypothesis:AADPR_125 Size=7215 b... | 4 |
| Row2 | Hypothesis:AADPR_143 Size=7034 b... | 4 |

Column containing Hypothesis: Hypothesis

Column containing matches: Minimum match number

Screen Source

Screen structures in: File Remote database

Column containing structures to screen:

File name: knime://knime.workflow/input/PhaseDB50.phdb Browse...

Output only: Maestro CT

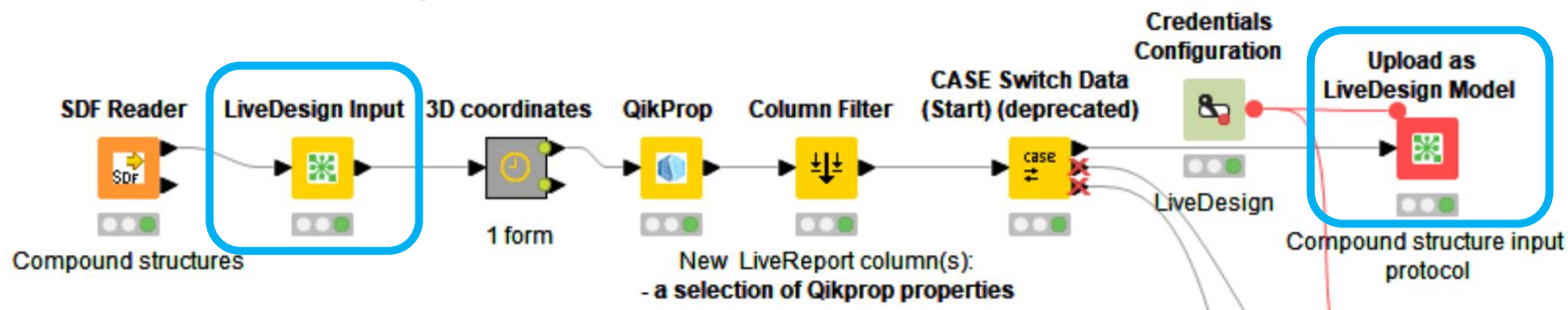
☒ Include log in output

Settings...

- In Maestro, KNIME menus under Scripts are planned to be retired
 - The menus are now hidden under a feature flag
 - Contact us if running KNIME workflows from Maestro is key for your work
 - We now recommend deploying KNIME models in LiveDesign to give your colleagues access to your workflows

Automatic protocol choice in the Upload as LiveDesign model node

- Automatic protocol choice
 - Set the LiveDesign protocol field to Same as current
 - Uses the protocol version in the installation
 - The node decides between the Compound structure and column input protocol based on a flow variable to created by the LiveDesign input node depending on its input (ID + sdf column vs. ID + other coumn(s)).
 - The protocol template is also chosen automatically in the Upload as LiveDesign protocol node
- Protocol deployed with the model
 - The protocol is installed automatically if it isn't already on the LiveDesign machine
- Coporate ID column
 - By default the first string column in the input table is used



No need to configure the Upload as LiveDesign model

- No need anymore to check the KNIME generic protocols are installed
 - And the most recent version is used
- No node configuration needed anymore
 - Using the usual settings stored in the KNIME preferences
 - Still configurable for some specific cases
 - eg testing on another machine before deploying on the production machine

This dialog box contains the following settings:

- LiveDesign host: From the Preferences
- Schrodinger Suite: From the Preferences
- LiveDesign project: From the Preferences
- Folder: (empty dropdown)
- LiveDesign protocol: Same as current
- Corporate ID column: Molecule name
- 3D column type: Ligands
- Command type: Normal
- ☒ Overwrite Model ☐ Preserve Model Data
- PyMOL script: (empty text area)

The 'Schrödinger' section of the preferences is shown with the following settings:

- Open Office spreadsheet command line: (empty text field)
- LiveDesign preferences: (checkbox, checked)
- LiveDesign host: <https://appsci-ld.onschrodinger.com>
- Schrodinger installation on the LiveDesign host: /mnt/squashsuites/suite2022-4-build082
- LiveDesign Project (if not found, fallback is 'KNIME' and then 'Global'): KNIME
- LiveDesign Base Folder for Models: Computational Models/KNIME/Test/22-4/



KNIME model calculation distribution

- The primary calculation host can be changed on the model Admin page
 - Use case: run computationally expensive steps on a virtual cluster accessible from the LiveDesign machine
 - Typically when GPU required (eg Desmond)
- Use Job server
 - Now by default but it can be changed on the Admin page
 - The calculations can be tracked with the Job manager tool in LiveDesign
- Job server debugging information
 - Reported on the Tasks page

VISUALIZE + Job Manager

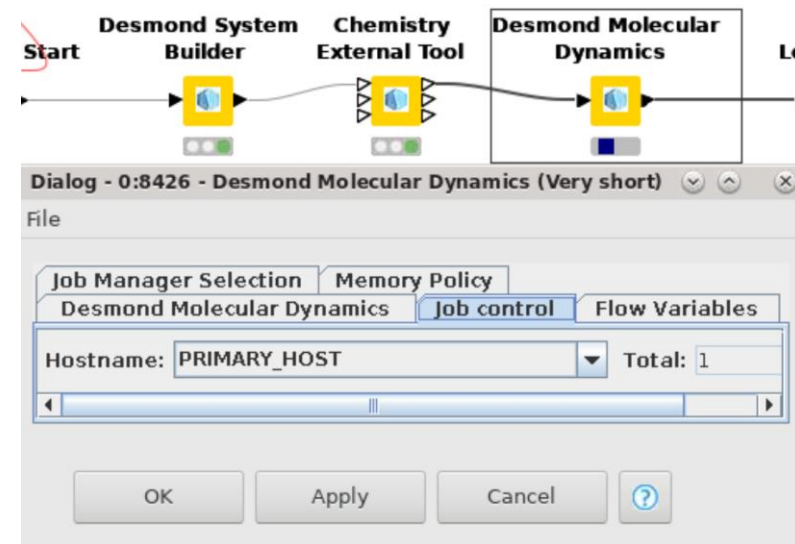
Use filters to locate jobs. Double-click for job details, right-click for additional actions.

| | | | |
|--------------------|-----------------------|-------------|-----------------|
| Launched by user: | Current user | Model: | All models |
| LiveReport: | Current LiveReport | Job status: | All |
| Compound Corp. ID: | (leave blank for all) | Submitted: | Any day or time |

| <input type="checkbox"/> | Compound ID | LiveReport | Model | User | Submitted | Status |
|--------------------------|-------------|--|-------|------------------------------|--------------|-----------|
| <input type="checkbox"/> | V181360 |  MD testing | Test | jean-christophe.mozziconacci | 19 Sep 14:57 | Completed |
| <input type="checkbox"/> | V223272 |  MD testing | Test | jean-christophe.mozziconacci | 19 Sep 15:01 | Completed |

KNIME model calculation distribution - example

- MD model example
 - Set the Desmond node in the workflow to run on the Primary host
 - In the KNIME preference the Primary host points to a local calculation cluster
 - Once the model uploaded change the Primary calculation host field on the admin page
 - Set it to a calculation cluster available from the LiveDesign machine



| | | | |
|--------------------------|-------------------------------------|--------|----------------------------------|
| Primary calculation host | <input checked="" type="checkbox"/> | STRING | Parent Data: localhost |
| | | | <input type="text" value="gpu"/> |

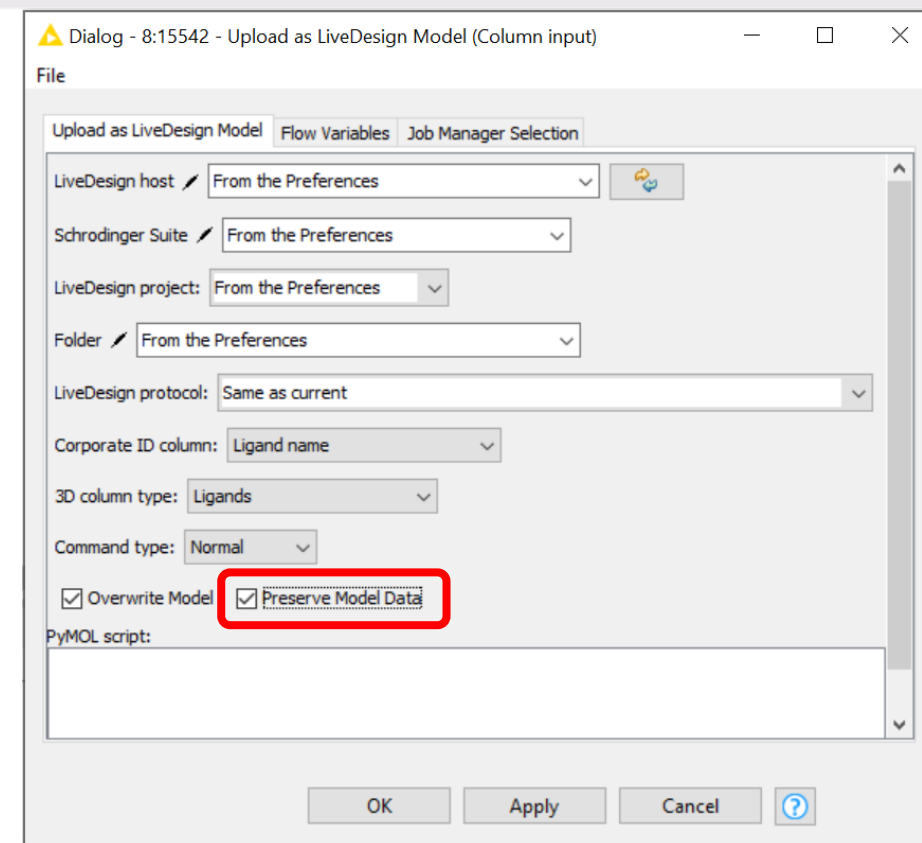
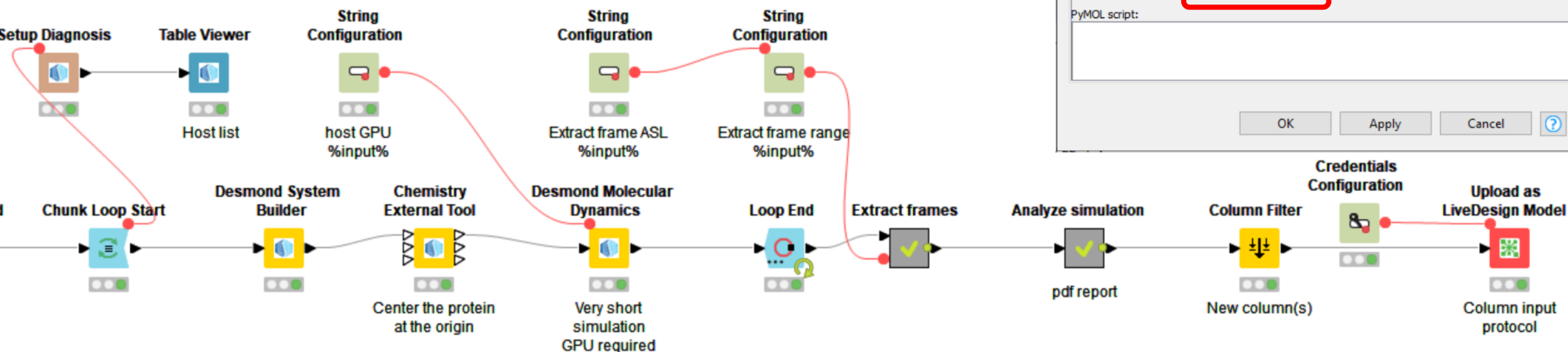
Upload as LiveDesign model – preserve existing model data changes

- **Scenario**
 - An initial version of the model was deployed
 - The model has been modified (settings or files) from the LiveDesign admin page
 - Then an improved version of the workflow has to be deployed
 - With the Preserve model data option, the model changes from the Admin page are preserved when overwriting the model
- **Off by default (advanced option)**
 - The node issue a warning and doesn't overwrite the model if the changes can't be preserved because the workflow has been significantly changed
- **Use cases:**
 - Keep the model settings set by a colleague (eg the number of conformers to keep or a system specific reference file) when updating the workflow with some improvements
 - Develop a workflow with some input structures or system and test it regularly in LiveDesign on another system a colleague works on
 - Test the workflow on a local calculation cluster and run the model on another cluster available from LiveDesign

Preserve Model data – use case

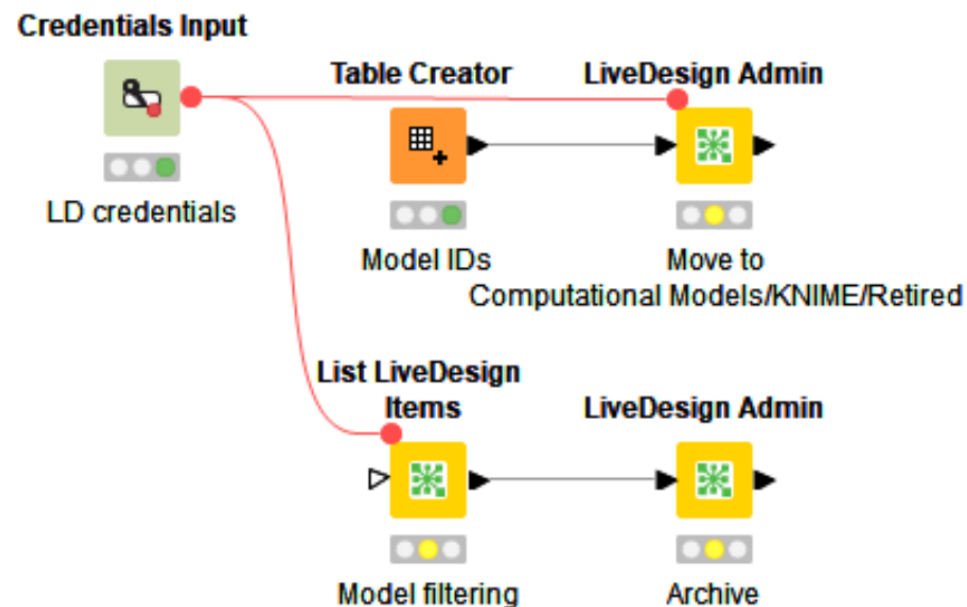
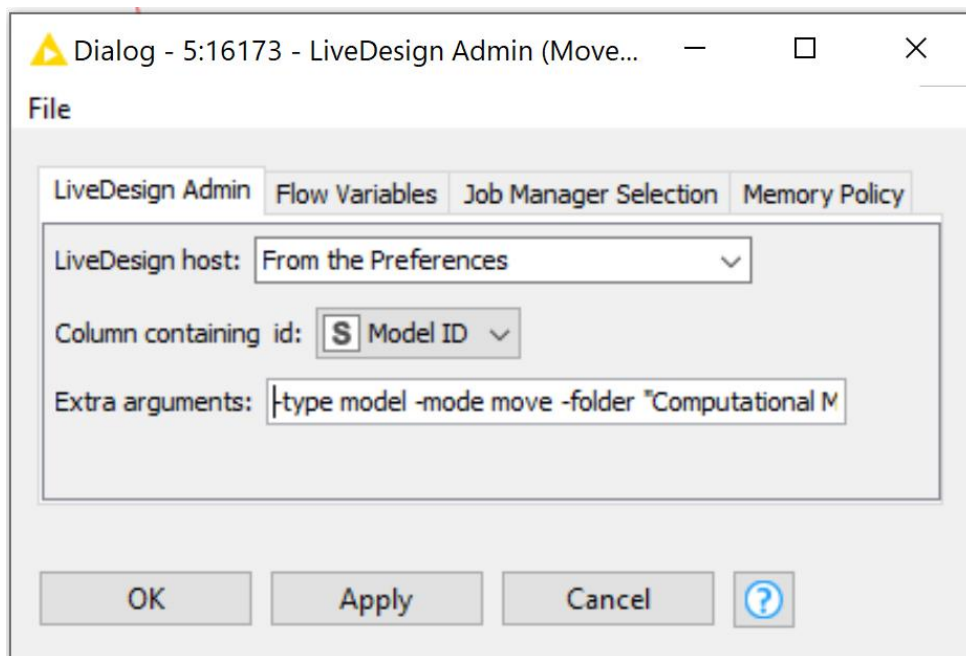
- Don't change the host to use on LiveDesign each time the model is updated

| | | | | |
|------------------|-------------------------------------|--------|--|-------------|
| extra argument 1 | <input checked="" type="checkbox"/> | STRING | Parent Data: -dummy -DesmondMD-HOST gpu | Set Fixed ▾ |
| extra argument 2 | <input checked="" type="checkbox"/> | STRING | Parent Data: -dummy -FrameRange '6::2' | Set Fixed ▾ |
| extra argument 3 | <input checked="" type="checkbox"/> | STRING | Parent Data: -dummy -FrameASL ligand | Set Fixed ▾ |



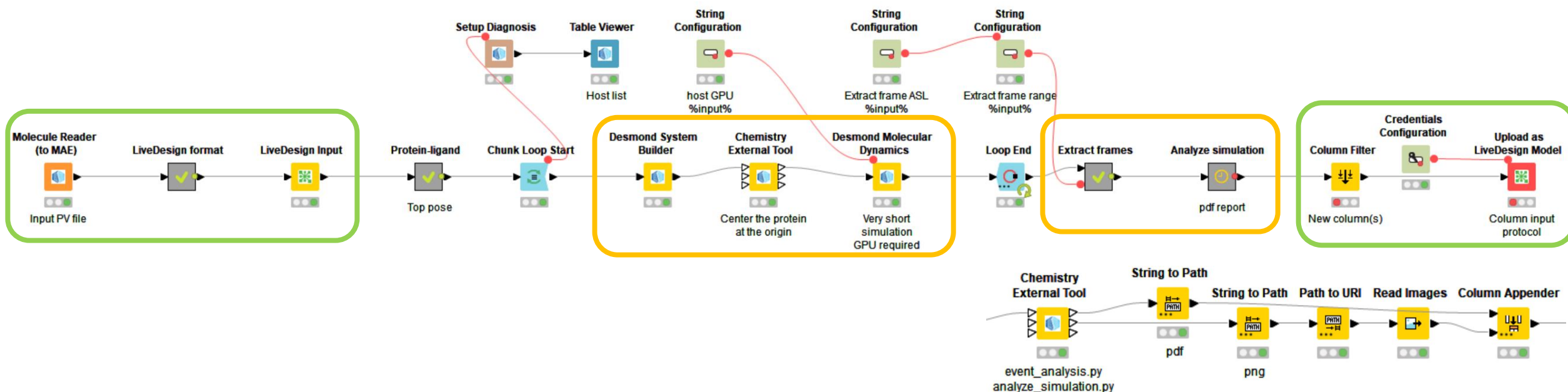
Model administration node

- Generic node to move, archive, unarchive models
 - One use case: archive a set of models before the corresponding protocol can be archived



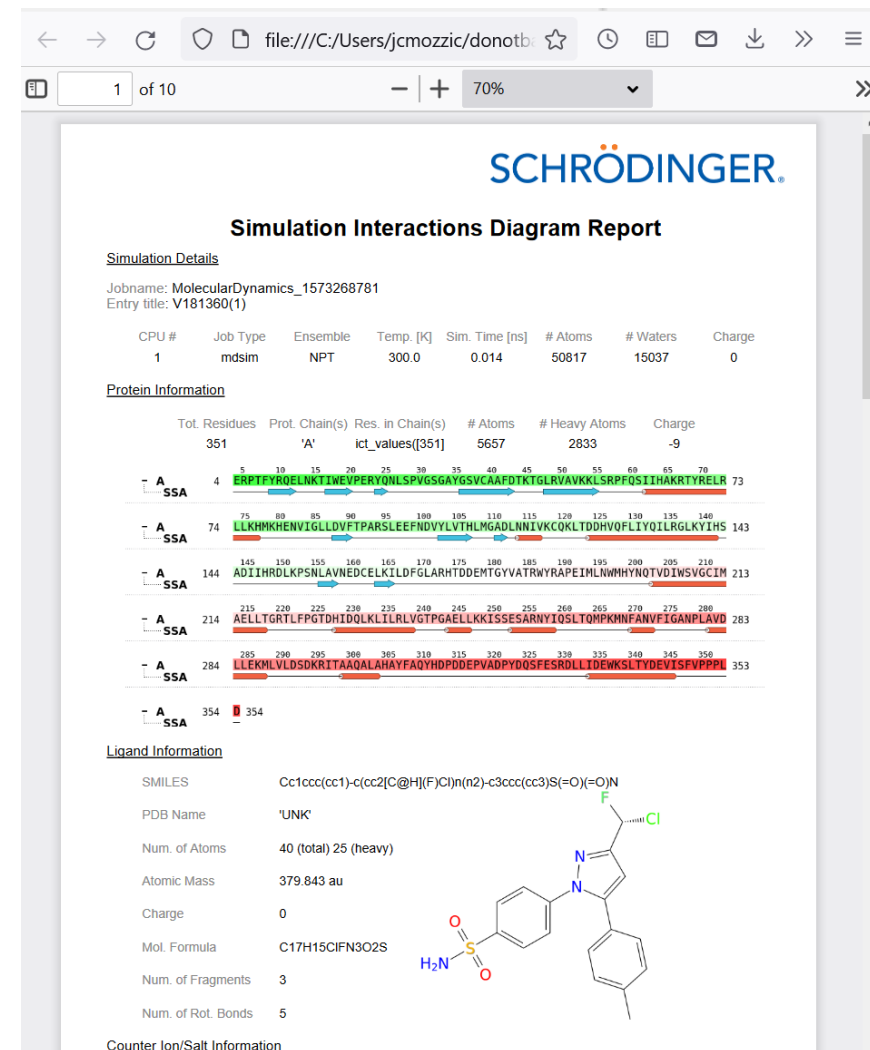
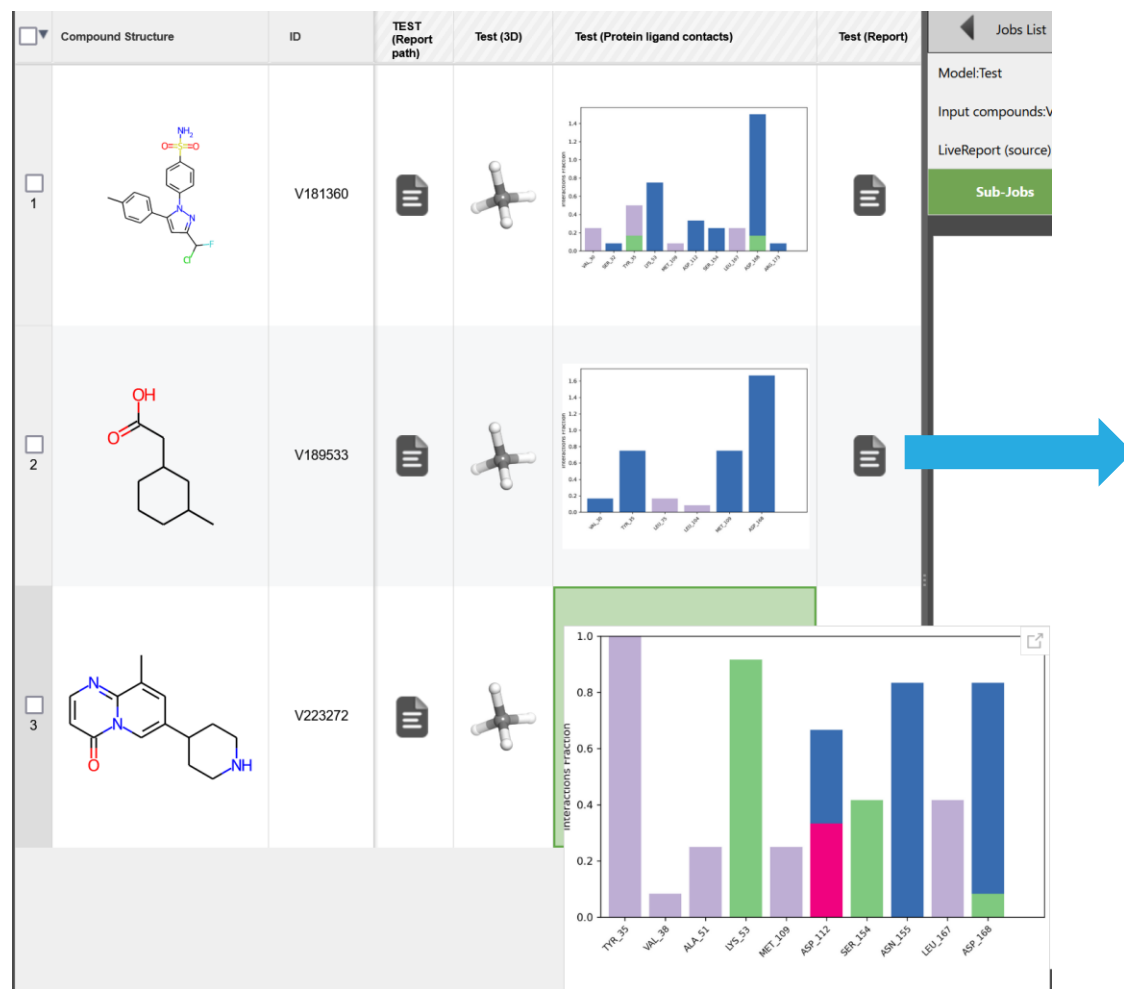
New and improved validated LiveDesign models

- Pharmacophore – Phase screening: with minimum match control
- Most of the validated models use the LiveDesign input node
 - To take advantage of the automatic protocol choice and installation
- Docking pose MD refinement and event analysis
 - Runs a molecular dynamics refinement on docking poses and generates an event analysis reports



New and improved validated LiveDesign models

- Docking pose MD refinement and event analysis
 - New columns in the LiveReport





New features in the KNIME extension

In Schrödinger Suite 2022-3

2022-3 New Features

- Schrödinger extension is compatible with KNIME 4.6
but it still includes KNIME 4.5
- Create and apply ML models with new DeepAutoQSAR nodes
- And minor improvements or fixes in the LiveDesign input, Upload as model and Blast nodes

KNIME Analytics Platform 4.6 – some new features

Highlights

- KNIME Modern UI Preview (Labs)
- New Visualization Nodes in KNIME (Labs)
- Bundled Python Environment
- Pure-Python KNIME Nodes (Labs)
 - Simple nodes can be written completely in Python
- Snowflake H2O Machine Learning Model Push-Down

Main improvements

- DB Framework Enhancements
- Microsoft Azure Services
- Column Expression and Multi-Row

Formulas

- Column Expressions is an all-purpose tool to compute new columns based on simple expressions. Multi-row formulas are now supported. Easier to manipulate and create path cells and variables.

- XGBoost

- Row weights control to remedy class imbalances or to prioritize certain subsets
- Bit & Byte Vector Support: for vector representation of the data which is common in life science
- Feature Importance Output of the XGBoost Tree Ensemble Learner nodes is an output table with various metrics that indicate how important every single feature is to the learned model.

- Extended Spark Support

See details in <https://www.knime.com/whats-new-in-knime-46>

KNIME Analytics Platform 4.6 – Pure-Python KNIME Nodes

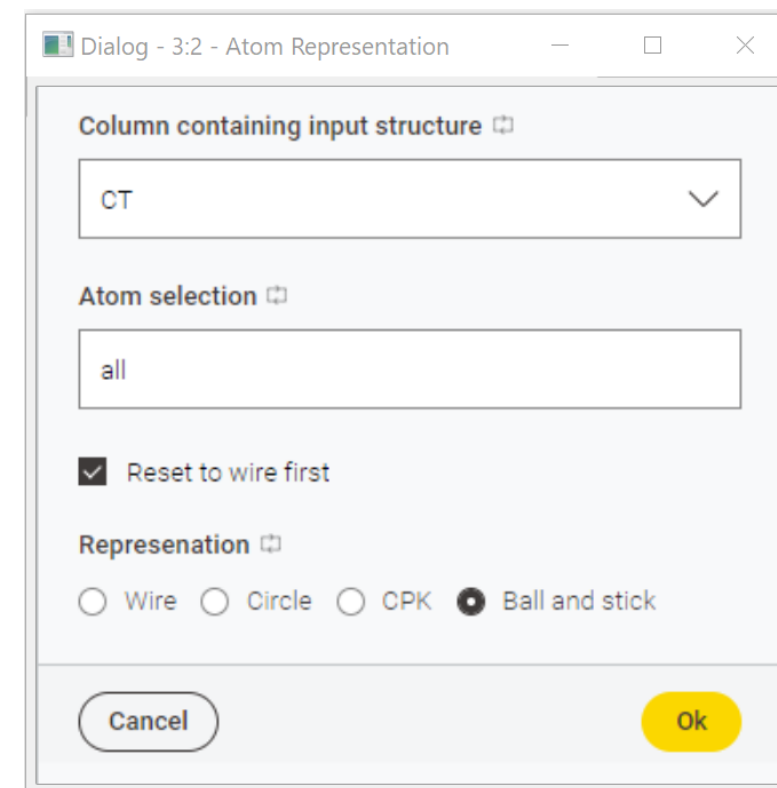
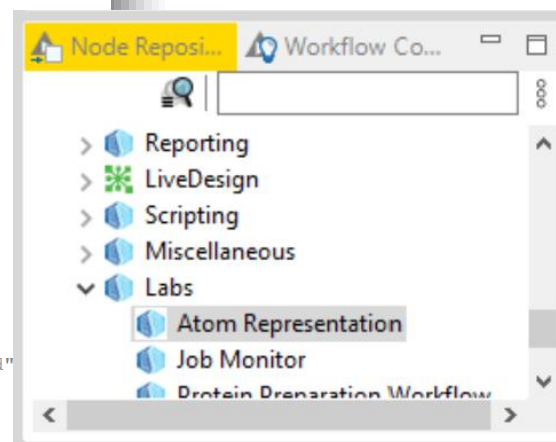
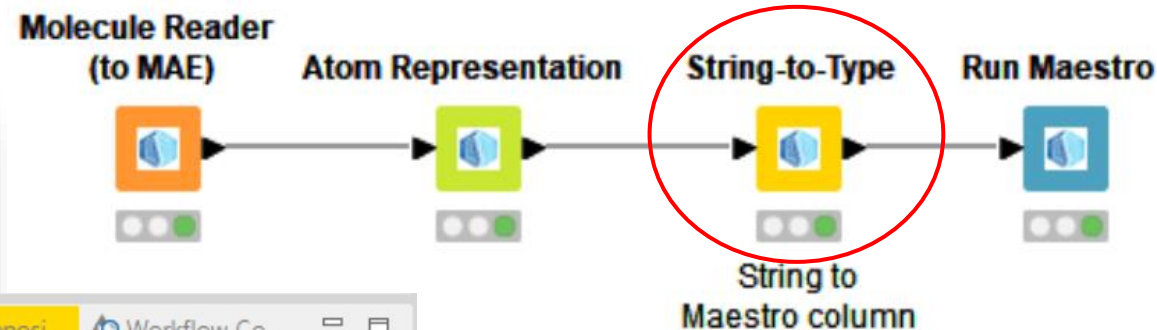
- Python node
 - The configuration panel and node functionalities are coded in 1 python file
 - Can be shared through an update site/zipped update site
- Current limitations (in Labs)
 - No chemistry output column
 - Workaround using a downstream string to sdf conversion node
 - Only simple configuration panel
 - Even compared to configuration nodes in a wrapped metanode
 - A KNIME development environment is required
 - To create the node and the corresponding update site
 - Schrodinger python libraries can't be used
 - Only python 3.9 is supported
 - But the node can execute a python script with \$SCHRODINGER/run
 - Schrodinger installation path must be set as environment variable, not only in KNIME preferences
 - Zipped update site size
 - Python installation embedded to avoid dependencies

- Usage
 - For node developers and nodes with simple configuration
 - Easy development of simple nodes
 - eg structure manipulation, atom representation...
 - Probably need to wait for improvements
 - Alternative
 - Chemistry external tool or Python node with some configuration nodes in a wrapped metanode
 - But can't be shared via an update site

KNIME python script available in the installation under:
knime_4.6.0/plugins/org.tutorial.<first_extension_0.1.0.202206301351>/src/main/python/<my_
extension>.py

KNIME Analytics Platform 4.6 – Pure-Python KNIME Nodes

Prototype example:



```
import knime_extension as knext

LOGGER = logging.getLogger(__name__)

@knext.node(name="Atom Representation", node_type=knext.NodeType.LEARNER, icon_path="schrodinger.p...")
@knext.input_table(name="Maestro input", description="Maestro input")
@knext.output_table(name="Appended String output", description="Maestro output as String column")
class TemplateNode:
    """
    Apply a representation to the selected atoms with an ASL.
    """

    NO_STYLE = "Wire"
    CIRCLE = "Circle"
    CPK = "CPK"
    BALLNSTICK = "Ball and stick"

    column_param = knext.ColumnParameter(
        label="Column containing input structure",
        description="Maestro input",
        port_index=0)

    asl_param = knext.StringParameter(
        "Atom selection",
        "ASL to specify the list of atoms to which the representation will be applied",
        "all")

    reset_param = knext.BoolParameter(
        "Reset to wire first",
        "Reset all atoms to wire before applying the representation",
        True)

    repr_param = knext.StringParameter(
        "Representation",
        "Select the atom style",
        NO_STYLE,
        enum=[NO_STYLE, CIRCLE, CPK, BALLNSTICK])

    OUTPUT_COLUMN_NAME = 'Output'

    def execute(self, exec_context, input_1):
        input_1_pandas = input_1.to_pandas() # Transform the input table to some processable format

        _, input_file = tempfile.mkstemp(prefix='AtomRep_', suffix='.mae', dir=os.getcwd())
        output_file = os.path.splitext(input_file)[0] + '_out.json'

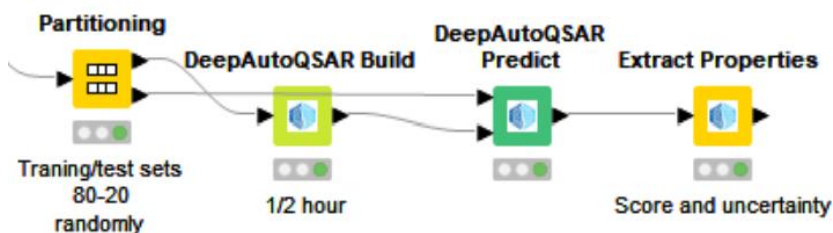
        LOGGER.info(f'Input file:{input_file}')
        LOGGER.info(f'Output file:{output_file}')

        with open(input_file, 'a') as writer:
            writer.write(self.MAESTRO_HEADER)
            for st_dict in input_1_pandas[self.column_param]:
                st_bytes = st_dict['0']['1']
                st_str = self.getStFromBytes(st_bytes)
                writer.write('\n' + st_str)

        cmd = [os.path.join(os.getenv('SCHRODINGER'), 'run'),
               '-FROM', 'knime', 'atom_style.py', input_file, output_file,
               '-style', self.repr_param, '-asl', self.asl_param,
```

DeepAutoQSAR build and predict nodes

- Same configuration panel as in Maestro
 - Including the report and scatter plot with uncertainties



AutoQSAR/DeepChem - Build

Options:

Model type: ☐ Classification ☒ Regression (numeric)

Prediction property: Select property... Add Descriptors

Training set: Random split 80%

Log transform: ☐

Training time: 0.5 hours

Set sizes: 787 training, 197 holdout, 984 total

OK Cancel

Dialog - 5:15633 - DeepAutoQSAR Predict

File

Flow Variables Job Manager Selection Memory Policy

DeepAutoQSAR Predict Job control

Column containing input : CT

Column containing QSAR Model: QSARModel

Output replaces Input Maestro ☐ CT

Settings...

OK Apply Cancel

AutoQSAR/DeepChem - Predict

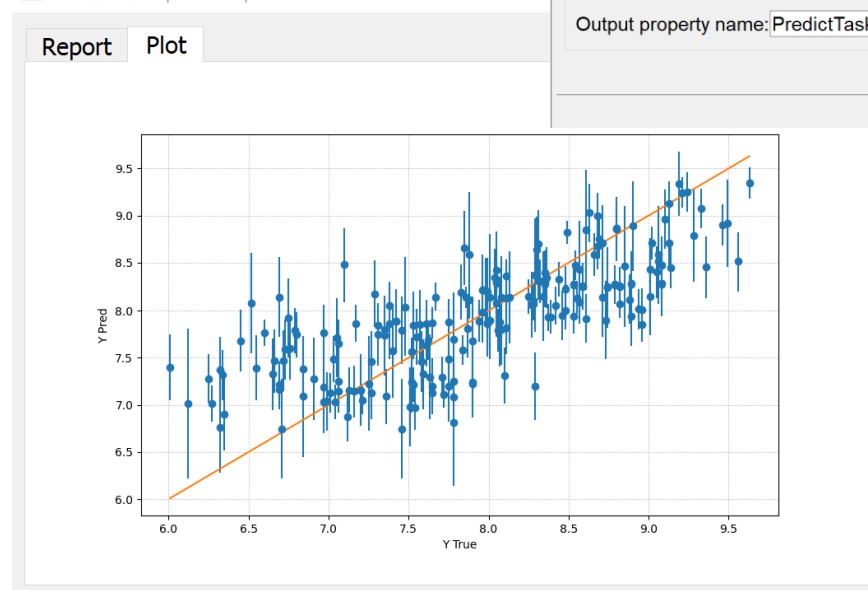
Model Summary

Mode: Regression
kendall_tau: 0.5733
mae: 0.4245
median_ae: 0.3610
r2: 0.5711
rmse: 0.5416
time: 2022-05-23-11-45-39-288

Make Predictions

Output property name: PredictTask

AutoQSAR/DeepChem Report Viewer



AutoQSAR/DeepChem Report Viewer

Report Plot

```
{
  "Mode": "Regression",
  "best": [
    {
      "models": {
        "165329225553645": {
          "additional_features": [],
          "atomic_mode": false,
          "dense_layer": 128,
          "dropout": 0.0,
          "epochs": 61,
          "featurizer": "Geometric_c",
          "layers": [
            64,
            64
          ],
          "learning_rate": 0.001,
          "learning_rate_schedule": "custom",
          "metric": "r2_score",
          "mode": "regression",
          "model": "TorchGraphConv",
          "num_features": 78,
          "num_tasks": 1,
          "results": {
            "score": 0.4506802591877143,
            "std": 0.03173236188897328
          },
          "transformers": [
            "norm"
          ]
        }
      }
    }
  ]
}
```

DeepAutoQSAR build – model saving option

- Save the QSAR models in the workflow
 - Default (KNIME philosophy)
 - But each model file adds 50-100M to the workflow size
- Don't save the QSAR models
 - eg when testing various scenarios
 - QSAR writer node to save the best model(s) on disk
 - Control the file name with the QSAR model name
 - The model files are deleted from the temporary when KNIME is closed

DeepAutoQSAR Build Job control Flow Variables Job Manager Selection Memory Policy

Column containing input : CT

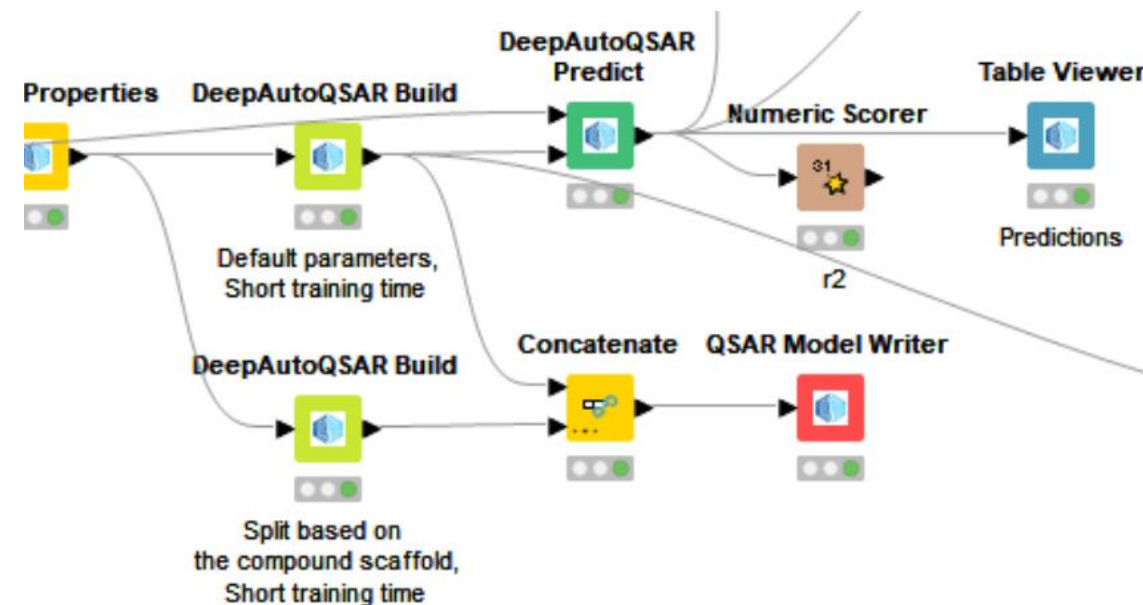
Output only QSARModel

QSAR model name: Scaffold split - 80% If empty, an unique name will be used

☒ Save model in output table

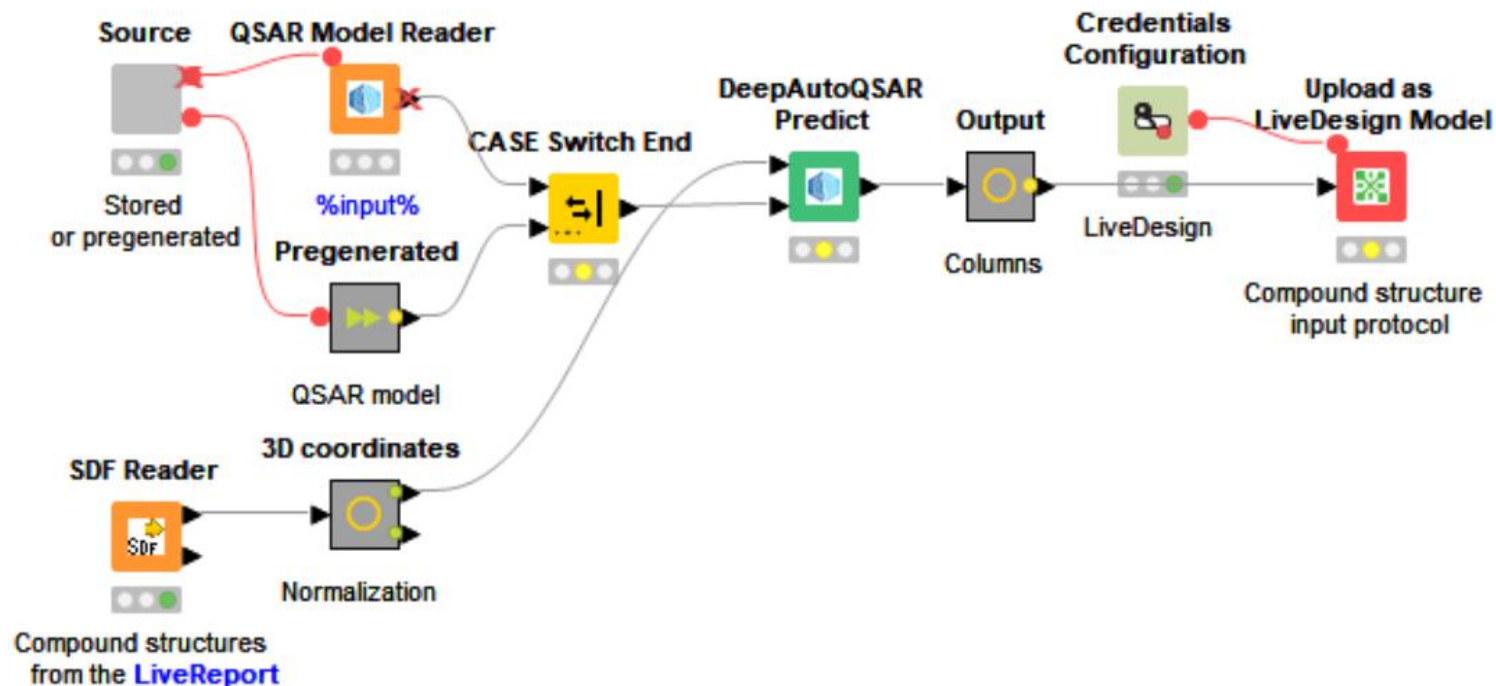
Settings...

OK Apply Cancel ?



New validated LiveDesign models

- DeepAutoQSAR: build and use models for predictions
 - The workflow can also be deployed as LiveDesign model





New features in the KNIME extension

In Schrödinger Suite 2022-2

2022-2 New Features

- Includes the latest version of KNIME (v4.5.1)
- New LiveDesign input node makes it easier to create KNIME models taking input columns from LiveDesign and store testing scenarios

The models based on the LiveDesign Column input protocol can now take 3D column(s) as input

- The Import from LiveDesign node preserves LiveReport column order
- Move models in bulk between folders for streamlined administration
 - e.g., to retire some models, rename a folder

KNIME Analytics Platform 4.5 – some new features

Highlights

- More Connection & Convenience
 - New Excel Cell Updater node and Excel Writer node improvement
 - New connectors for standard file systems
- New & Improved Deployment Possibilities
 - Workflow services make it much easier to call KNIME workflows from other workflows
 - Enhanced Dynamic Data Apps: new re-execution capabilities in widgets
- Integrating Python & KNIME

Notable Improvements

- Faster Workflow Execution
- Authentication Enhancements

Smaller Updates

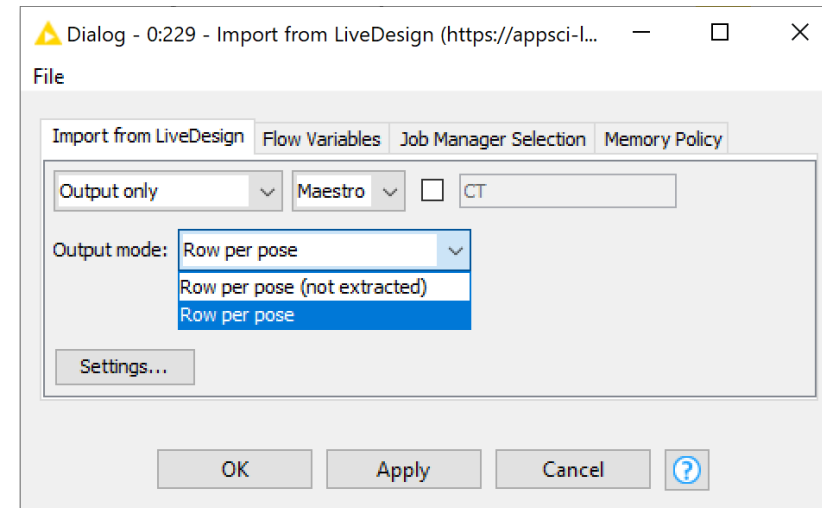
- KNIME Hub Improvements
 - Search Filtering by Tag on the search page, lets you filter the results based on one or several tags
 - As-you-type results
 - Recent search
- New Learner Nodes for Regressions
- Dynamic Ports in Switch & Loop Nodes
 - Switch & Loop nodes now support dynamic ports. As a result, nodes such as the CASE Switch Start support more port types. Loop nodes, such as Loop End, can now be customized to support multiple inputs



See details in <https://www.knime.com/whats-new-in-knime-45>

The Import from LiveDesign node output looks more like the LiveReport

- Extract all the LiveReport columns
 - Alternatively it can be stored as structure properties and extracted when necessary
- In the same order as in the LiveReport
 - The output table contains 1 row per pose
 - Same as when imported to Maestro
 - The poses can also be grouped
 - So that the table looks similar to the Row per compound LiveReport view



Workflow diagram: LiveDesign Connection → Import from LiveDesign → Group poses → Filtered table - 0:15236 - Column Filter

| Row ID | SMILES | ID | Docking... | Ensemb... | Low energy conformations (3D) | Test (Dihedral angle) | Ensemble docking (3D)->V181360 |
|--------|--------|---------|------------|-----------|-------------------------------|---|---|
| Row0 | | V181360 | #CTs: 2 | -5.7 | #CTs: 20 | Pose 1: 154.2 Pose 2: 44.3 Pose 3: 44.3 Pose 4: 154.2 Pose 5: 154.2 Pose 6: -154.2 Pose 7: -154.2 Pose 8: 154.2 Pose 9: -154.2 Pose 10: 44.3 | Molecule: V181360 (pose 1320315) #atoms:... |

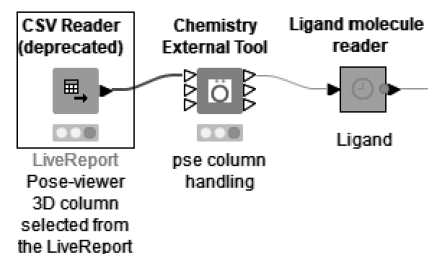
- Improved layout of the cells with multiple values (e.g., docking scores)
 - Using the String-to-type node

Easier creation of KNIME models taking input columns

- **New LiveDesign input node**
 - Can take its input from files exported from LiveDesign if a LiveReport with suitable columns is available
 - Otherwise from an upstream workflow section
 - More convenient to store some testing scenarios
- **Column input protocol**
 - Can take several LiveReport columns as input, now including 3D columns
 - Using the LiveDesign input node
 - Only 2 generic KNIME protocols covering all the needs:
 - Compound structure input protocol: only the compound structures as input
 - Column input protocol: 1 or several input columns
 - Parametrized models
 - 1 column input protocol will be retired
(It uses the old mechanism based on the CSV reader node as input)

Easier model creation using files exported from a LiveReport

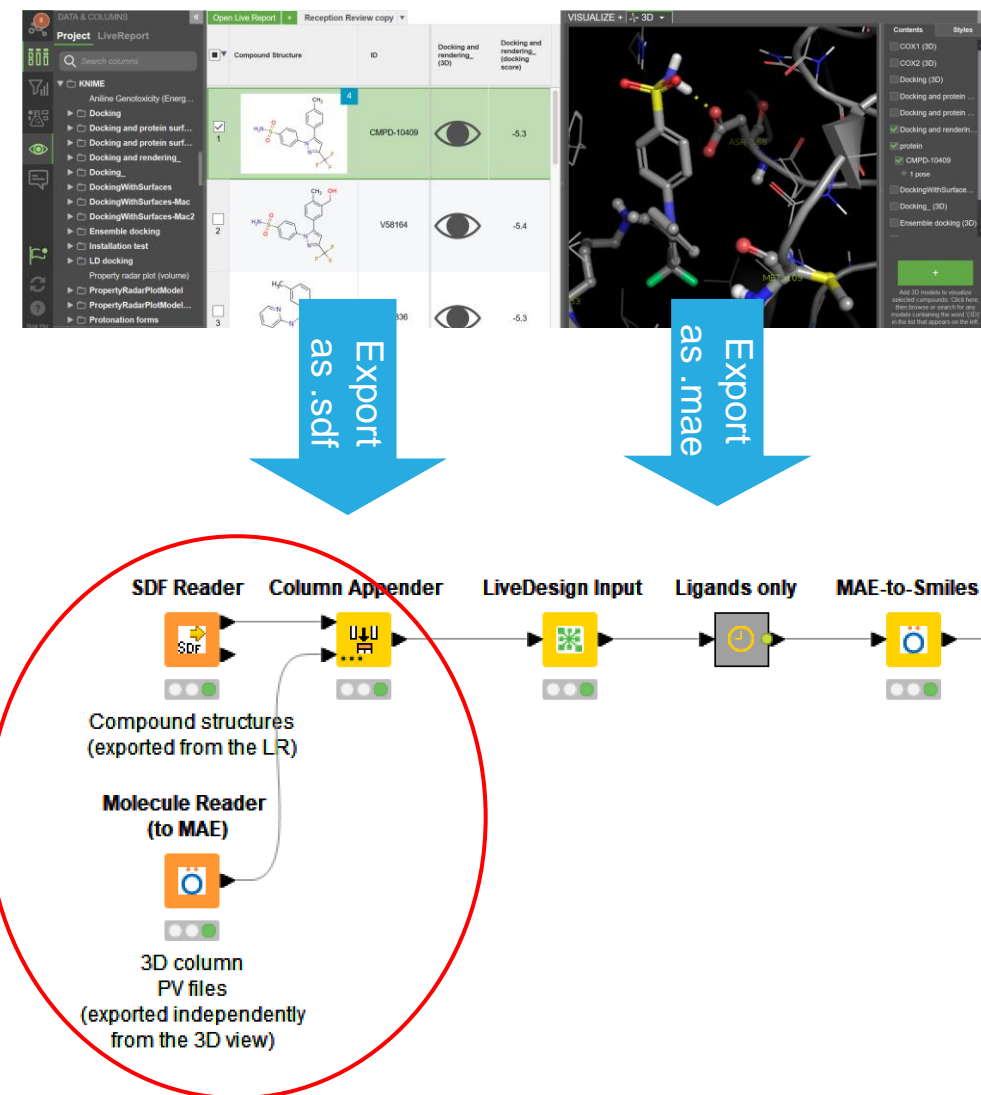
- Read files directly exported from LiveDesign
 - SD file export with the Compound structure
 - Or a CSV/Excel file with selected LiveReport columns
 - The column order must be the same as the selection order in the Parametrize model panel
 - Optionally file(s) exported from the 3D view with 3D column(s) data
- The node outputs the Compound structures and any selected columns
 - From the LiveReport when run in LiveDesign
 - Column name standardization
 - No need of a tag: this node is dedicated to take the LiveReport input



File Table - 7:452 - CSV Reader (deprecated) (LiveReport)

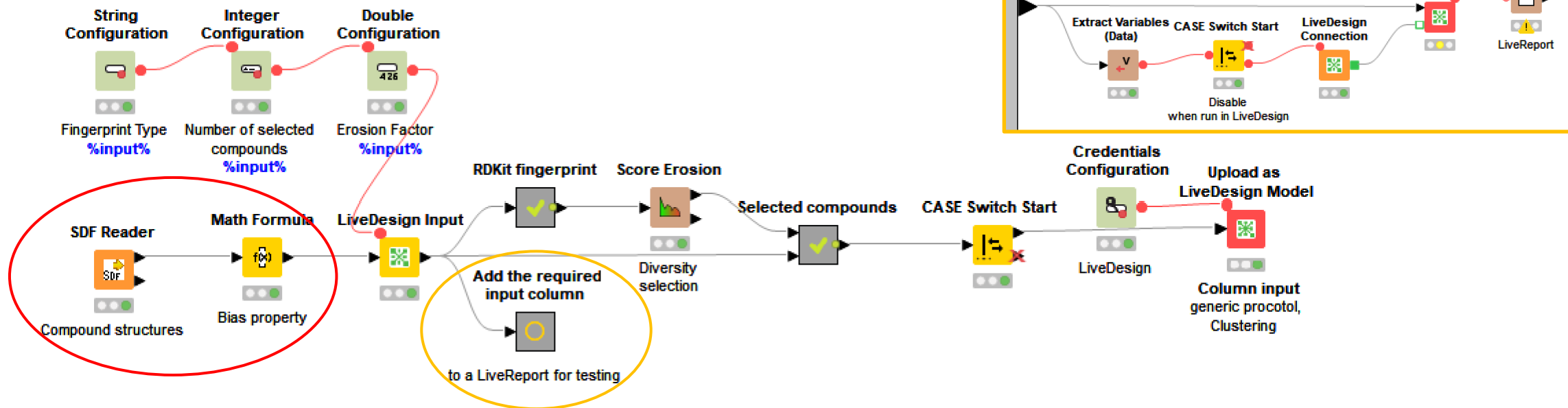
Table "Ligands.csv" - Rows: 3 Spec - Columns: 3 Properties Flow Variables

| Row ID | Corporate ID | Ligand | Protein |
|--------|---------------|--------------------------|--------------|
| Row0 | V222790 | Row0_2_Row0_48305646.mae | ? |
| Row1 | CHEMBL1766301 | Row1_2044625589.mae | Row0_1234... |
| Row2 | CHEMBL1766301 | Row2_1838273440.mae | Row0_1234... |



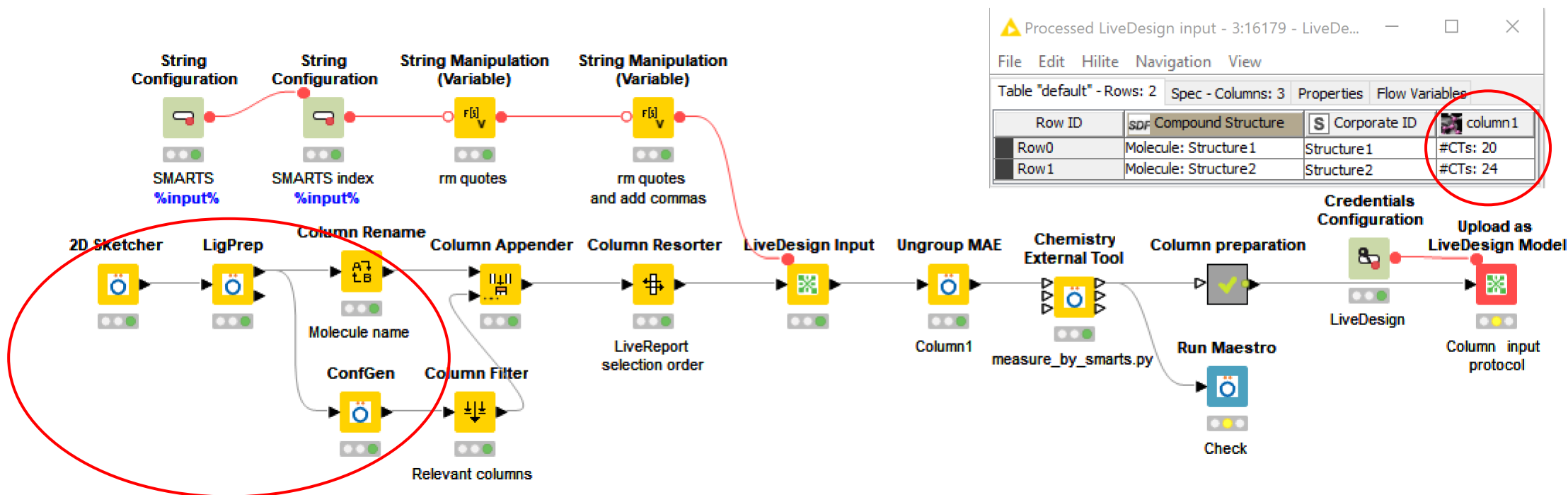
Easier model creation using the LiveDesign input node

- Upstream nodes to create and store a proper workflow input
 - Mockup of the selected LiveReport columns for prototyping
 - No need of a dedicated LiveReport to create and test the workflow
 - e.g., docking input section for the post processing models like the Binding pose strain model
 - Self-contained workflow
 - e.g., develop the model on a test LD machine where the real input data isn't available
 - Optional workflow branch to add the required input columns or create a LiveReport for testing
- eg Biased diversity section model:



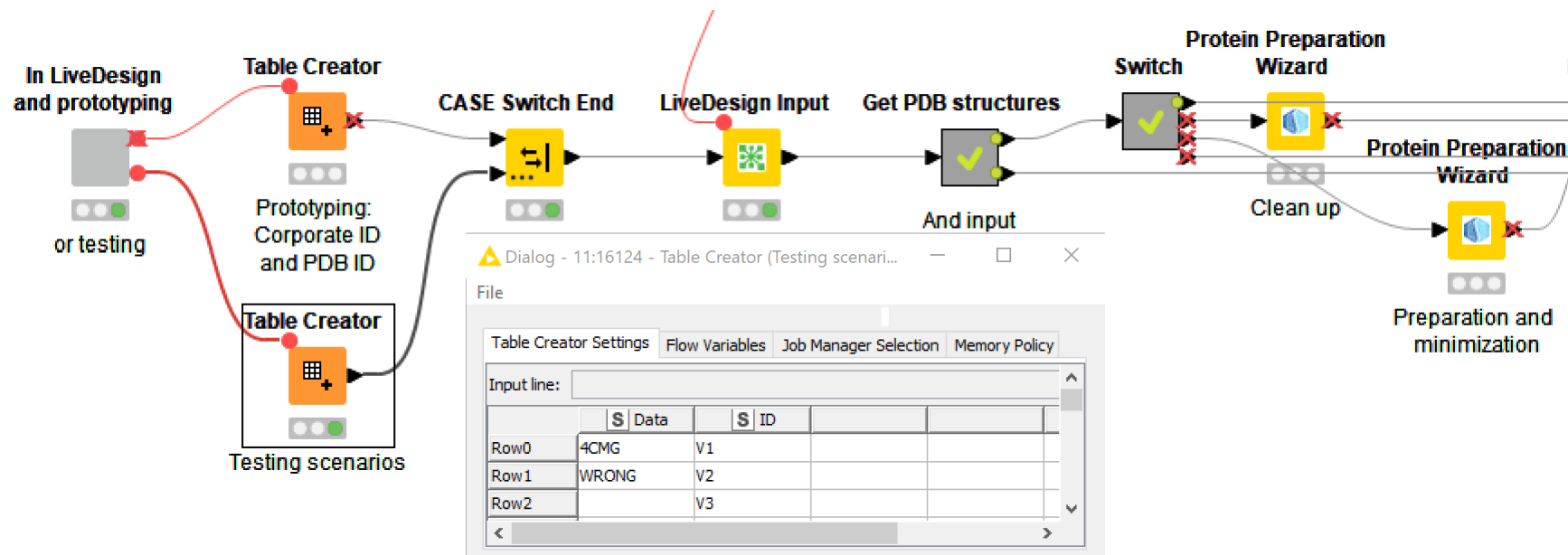
Model taking 3D column(s) as input

- Measure a dihedral angle model
 - Input: a 3D column with conformers
 - Dihedral angle definition
 - Defined with a SMARTS pattern common to the ligand series and atom indices in this pattern
 - Connect the Flow variable nodes to the LiveDesign input node
 - Input replaced by the LiveReport data when the model is executed in LiveDesign



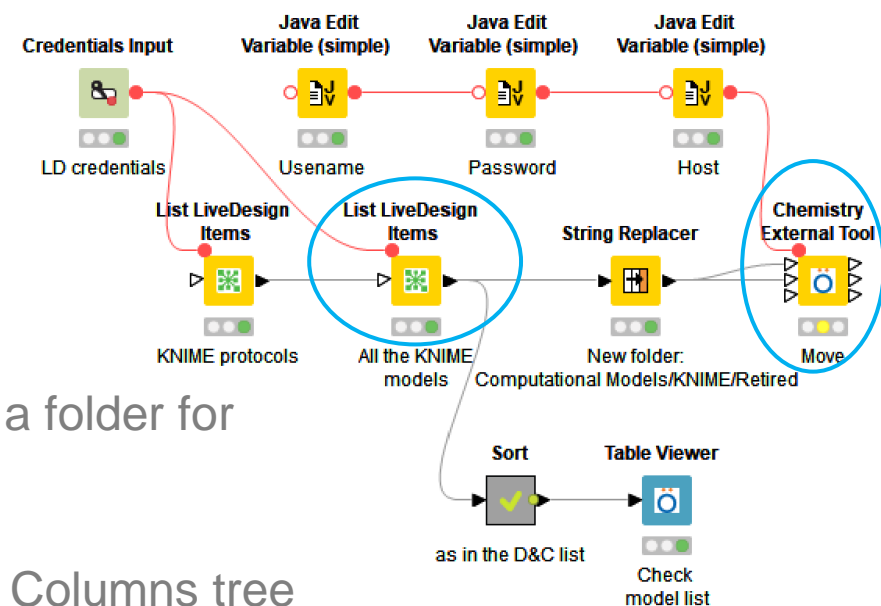
Testing scenarios in the workflow

- Create and store testing scenarios
 - As input to the LiveDesign input node
 - Testing the model on various scenarios
 - e.g., wrong, missing values...
 - Self-contained workflow
 - Testing data stored in the workflow instead of a dedicated LiveReport with the required input columns
 - e.g., Extract cocrystallized ligands and the Docking post processing models
 - Extend progressively



Model administration and deployment

- Move models in bulk to other folders
 - Through the command line. Instead of making the change on the Admin page for each of model
 - "\$SCHRODINGER"/run -FROM knime LiveDesign_admin.py
 - username <credential> -password <credential>
 - host <Host> -type model -**mode move**
 - id <list of IDs> -**folder** "<new folder>"
 - Application examples:
 - Clean up the Data & Columns tree by moving old models to a folder for retired models (before archiving)
 - In combination with the List LiveDesign item node
 - Rename a folder containing models. Reorganize the Data & Columns tree
- Upload a workflow as protocol from a workflow file
 - Using LiveDesign_admin.py
 - e.g., workflows from the KNIME hub ready to be uploaded
 - But they have been prepared to be uploaded either as model or protocol



Minor change

- The nodes have to be reconfigured if the input column has changed
 - Typically when the column was renamed or deleted
 - When rerunning workflows created with a previous release some nodes may now fail with a message like:
 - WARN AutoQSAR Predict 9:19 The column 'CT' does not exist in input specs
 - Usually opening the configuration panel before executing the node is sufficient
 - Possibly the input column would have to be selected again
 - Previously the nodes were using the first column of the same type as the best guess. But it could create confusion especially when the workflow is run in batch
 - And this is KNIME node standard behavior

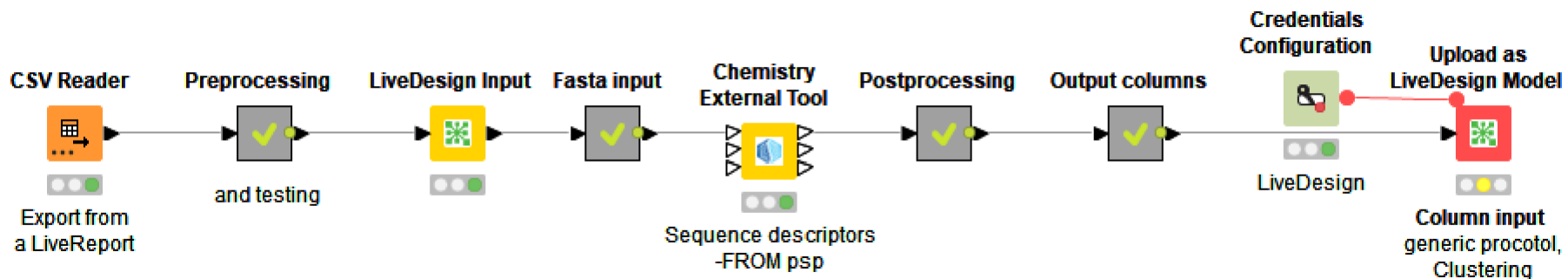
Workflow examples and validated LiveDesign models

Updated workflows and LiveDesign models:

- List models and protocols: move models in bulk
- LiveDesign import and export: extracted columns and grouped poses
- Chemoinformatics models – QSAR random forest: using RDKit descriptors
- LiveDesign models using the LiveDesign input node:
 - Binding pose strain, Biased diversity selection, Get PDB and preparation, Cocrystallized ligand

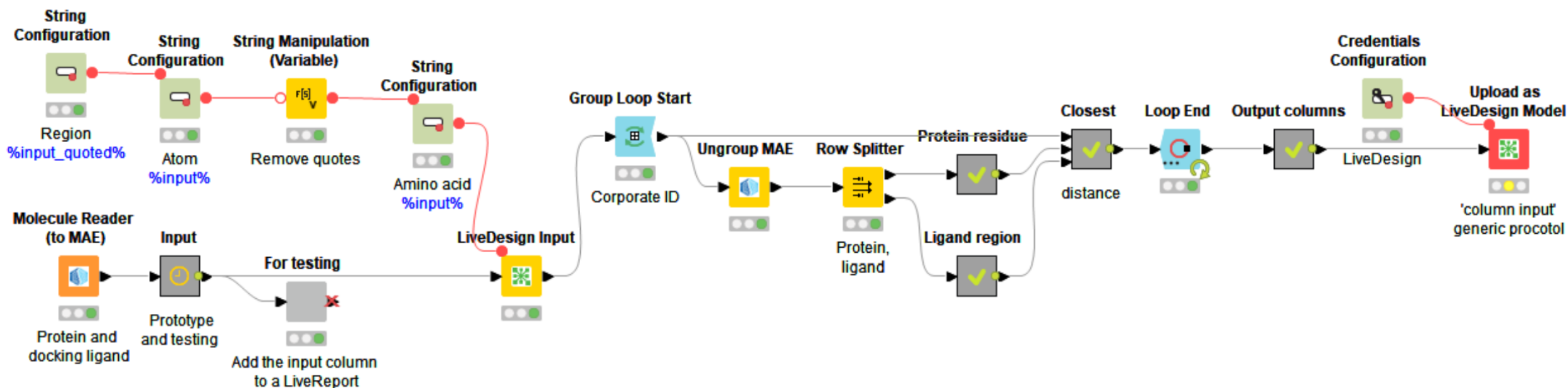
New LiveDesign models:

- Sequence descriptors: can run on a LiveReport with Generic Entities (no structure) since it takes a text column containing the protein sequence as input



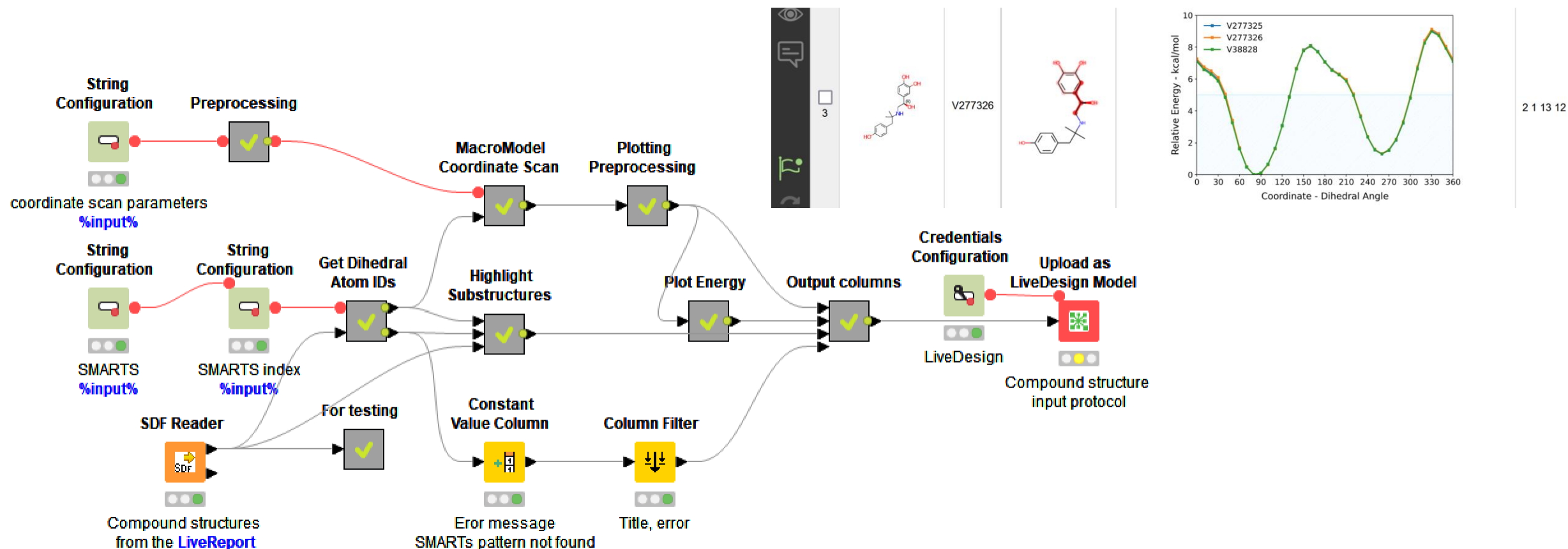
New validated LiveDesign models

- AutoQSAR prediction: including a model building section before the LiveDesign input node
- Measure dihedral: defined with a smarts pattern and atom indices
- Distance measurement: ligand – residue or between 2 sections of the ligand defined by smarts patterns



Workflow examples and validated LiveDesign models

- Torsion plot for a specific dihedral
 - KNIME, RDKit, python combination, run in LiveDesign





New features in the KNIME extension

In Schrödinger Suite 2022-1

2022-1 New Features

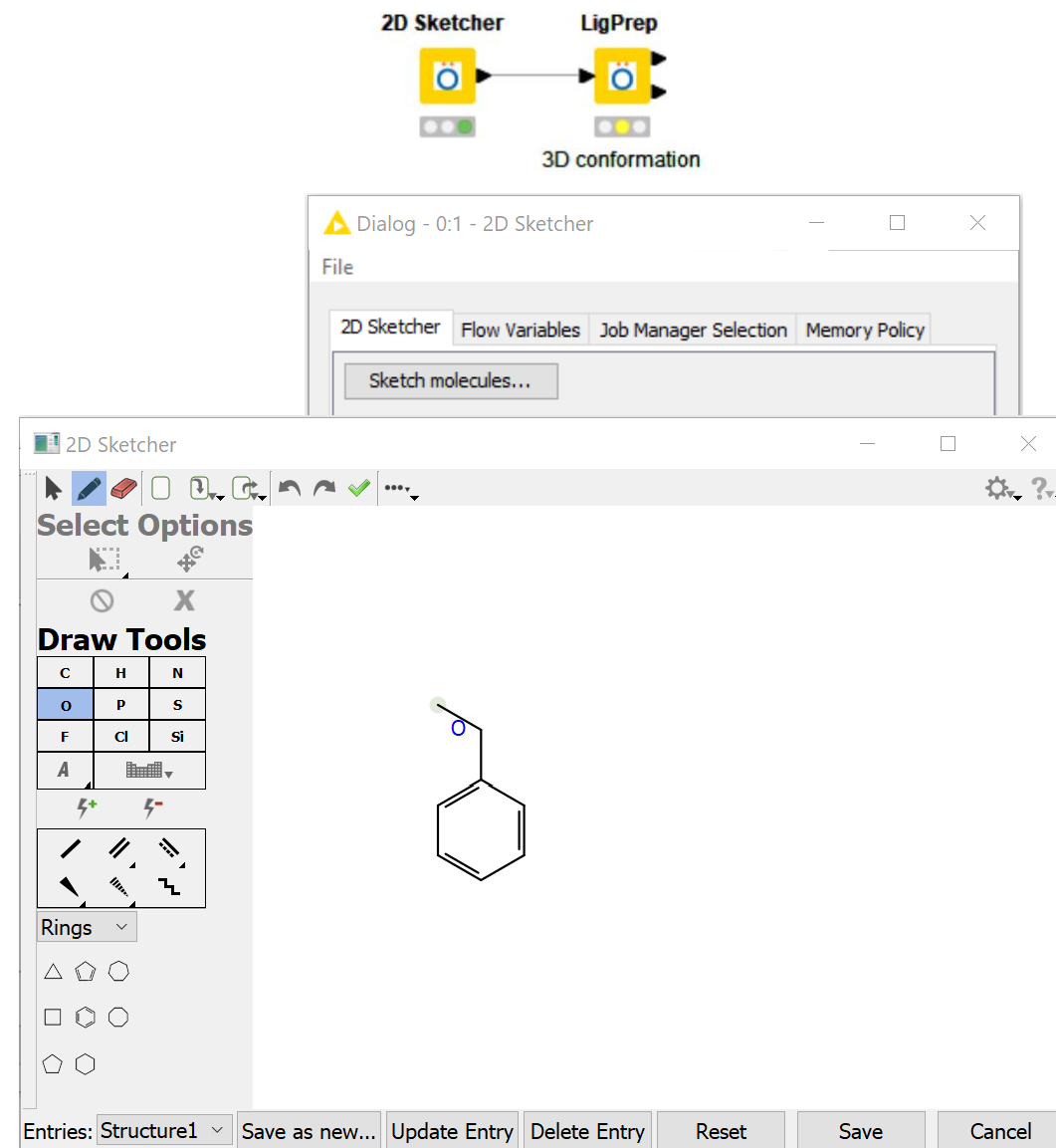
- New 2D Sketcher node

Run from LiveDesign:

- Export to LiveDesign node can export the whole table.
So model results can be stored in new LiveReport(s)
- The model output columns can contain files (eg with pdf)
- Store the executed workflow in a LiveReport column for easier debugging

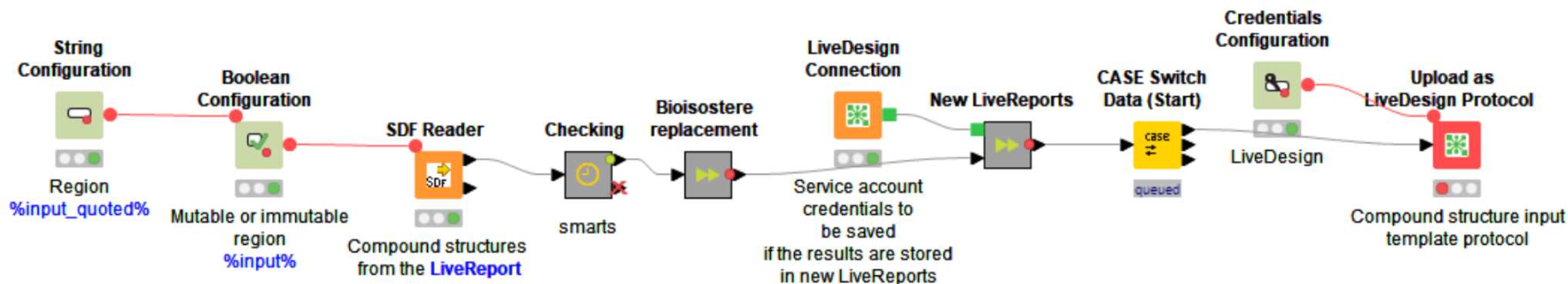
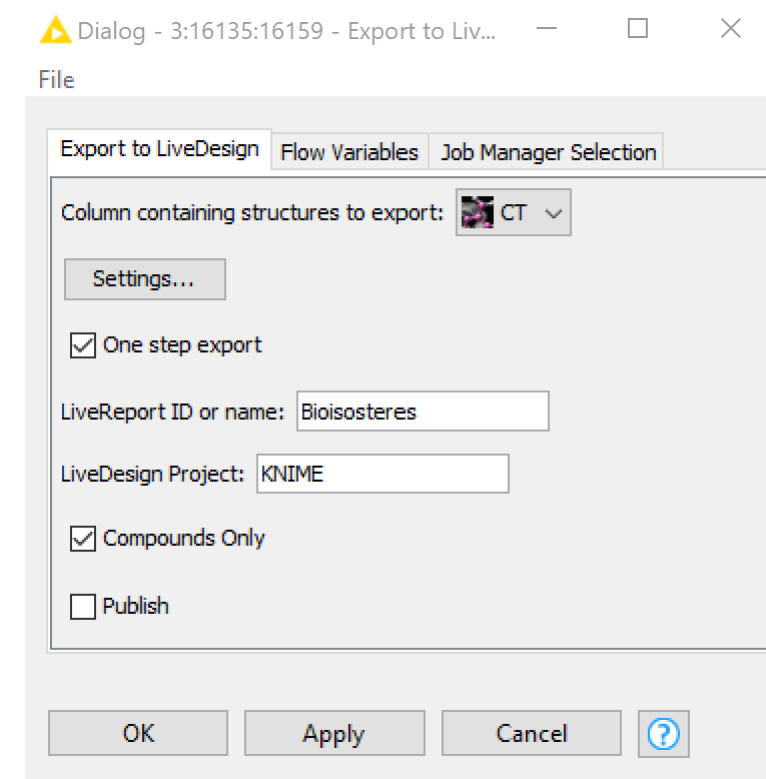
2D sketcher node

- Same as in Maestro and LiveDesign
 - Take advantage of the recent improvements
- Sketch 1 or several compounds
- Smiles output column
 - LigPrep node to turn structures in 3D
 - The reactions and substructures can't be stored yet

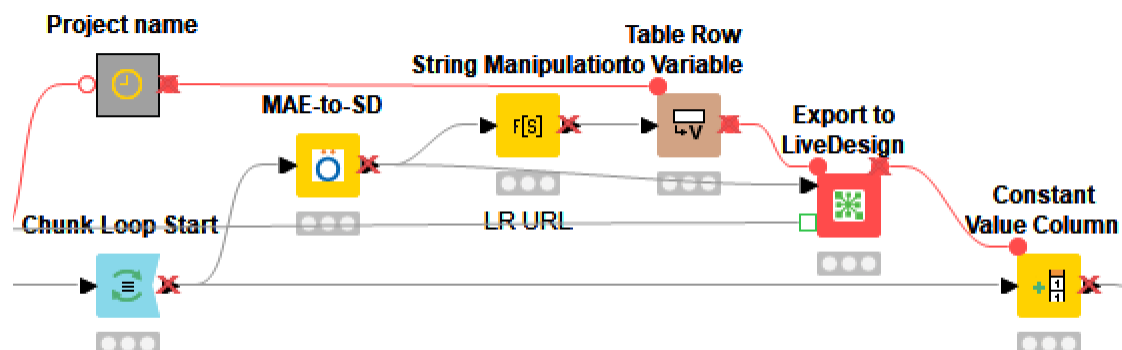


Export to LiveDesign – export all the columns

- One step export
 - No need to use the Maestro panel
 - No need to change the configuration if the column list has changed
- Use to store model results in new LiveReport(s)
 - Credentials have to be stored (encrypted) in the workflow
 - Application example: bioisostere replacement model
 - New LiveReports: for each set of bioisosteres
 - Easy result inspection, filtering, further usage in LiveDesign
 - Input LiveReport: new column with the links to the new LiveReports



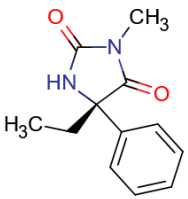
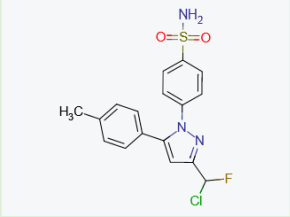
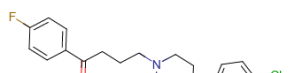
Bioisostere replacement – output in new LiveReports



Each bioisostere set
in a LR

KNIME Give Feedback

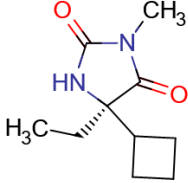
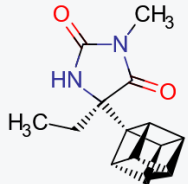
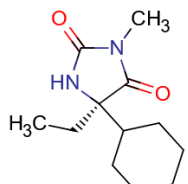
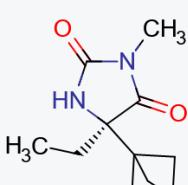
LiveReports... + Bioisostere replacement

| Compound Structure | ID | All (# bioisosteres) | All (New LiveReport) |
|---|---------|----------------------|--|
|  | V179296 | 21 | Bioisosteres for V179296 |
|  | V181360 | 43 | Bioisosteres for V181360 |
|  | V213806 | 53 | Bioisosteres for V213806 |



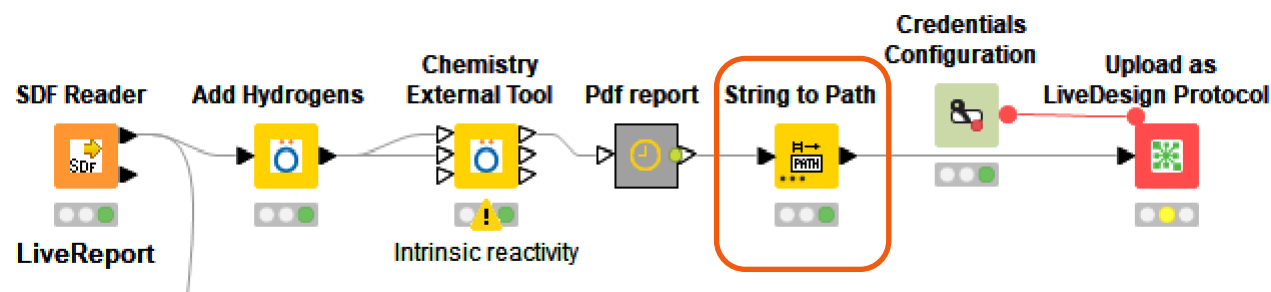
KNIME Give Feedback

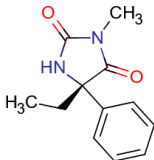

LiveReports... + Bioisostere replacement x Bioisosteres for V179296

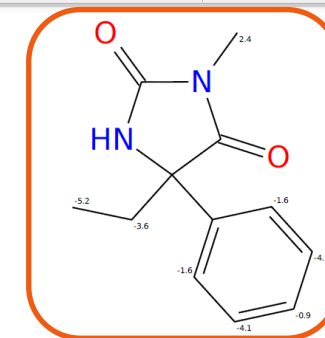
| Compound Structure | ID | All IDs | Ratio |
|---|---------|---------|-------|
|  | V221481 | V221481 | |
|  | V221482 | V221482 | |
|  | V221483 | V221483 | |
|  | V221484 | V221484 | |

Model output – file columns

- Create a new column containing files (eg pdf)
- Path type column from the input table, pointing to files written to disk by a node upstream. Corresponding columns with Other type.
- The Upload node model/protocol column management covers all the LiveDesign column types (except boolean):
 - String, real, integer, 3D structure, image, other (ie files)
- Application example: Site of metabolism model
 - `p450_results_gui.py -r -o report.pdf`



| <input type="checkbox"/> | Compound Structure | ID | SOM model (path) |
|--|---|---------|---|
| <input type="checkbox"/> 1 |  | V179296 |  |
| 1 Compounds · 0 Selected · 8 Columns (21 Hidden) | | | |



Model output – executed workflow

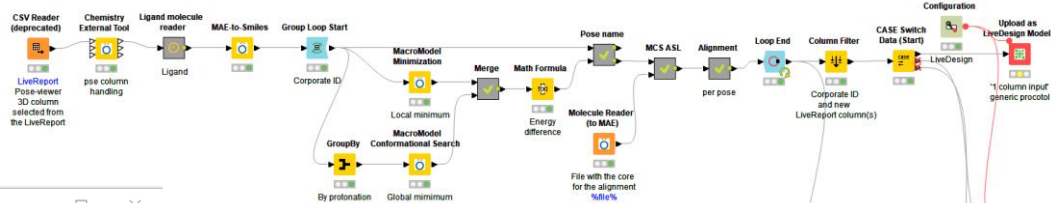
- The executed workflow file available for downloading in the LiveReport
 - Add a new column called 'Executed workflow' and type 'Other' in the Prediction section of the model page
 - Open the file in the KNIME GUI for debugging
 - Understand the results (eg scientifically)

Executed workflow

Executed workflow

Other (e.g. .pdf, .zip) ▼

+ Add Another Prediction



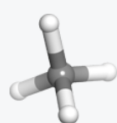



Filtered table - 3:479:451 - C...

| Row ID | Corporate ID | CT |
|--------|---------------|---------------------------|
| Row0 | V222790 | Molecule: 4CMG #atoms:... |
| Row1 | CHEMBL 176... | Molecule: V37754 #atom... |
| Row2 | CHEMBL 176... | Molecule: V37754 #atom... |

Concatenated table - 3:15403:15393 - Concatenate

| Row ID | Corporate ID | CT | Pose in... | RowID | Pose or... | D Global ... | D Local minimum energy |
|--------------------------|--------------|---------------------------|------------|--------------------------|------------|--------------|------------------------|
| V222790_binding_pose_1 | V222790 | Molecule: 4CMG #atoms:... | 1 | V222790_binding_pose_1 | 1 | ? | ? |
| V222790_local_minimum_1 | V222790 | Molecule: 4CMG #atoms:... | 1 | V222790_local_minimum_1 | 2 | ? | -190.93 |
| V222790_global_minimum_1 | V222790 | Molecule: 4CMG #atoms:... | 1 | V222790_global_minimum_1 | 3 | -190.935 | ? |

| Cocrystallize d ligands (3D) | Cocrystallize d ligands (Executed) | Cocrystallize d ligands (Ligand | Cocrystallize d ligands (Ligands by | Cocrystallize d ligands (PDB_ID) |
|---|---|--|--|--|
|  |  | 4QQ (1) | H(1) | 1ETT |
|  |  | S58 (4) S58 (4) S58 (4) S58 (4) | C(1), D(1), A(1), B(1) C(1), D(1), A(1), B(1) C(1), D(1), A(1), B(1) C(1), D(1), A(1), B(1) | 1CX2 1CX2 1CX2 1CX2 |
| | | | More available... | |

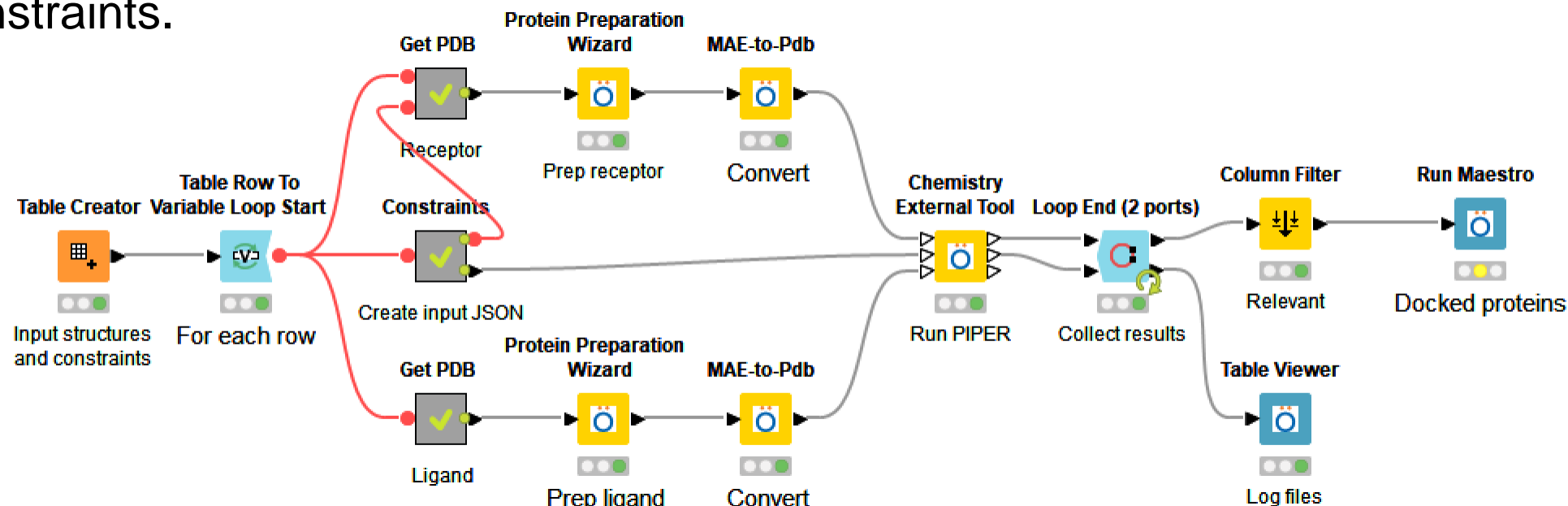
- If the task has failed the executed workflow is available from the Tasks page among the temporary files

Generic protocols

- Improved with a field to control environment variables:
 - eg canvas memory limit, Schrodinger temporary directory
- Simplified
- Reduced the default log verbosity
 - Error messages only
 - Download the executed workflow for further investigation

Workflow Examples and Validated models

- Docking – PIPER: runs PIPER docking to generate protein-protein complexes using constraints.



LiveDesign models:

- LiveDesign model – Bioisostere replacement: output in new LiveReports

Available on: https://hub.knime.com/schroedinger/spaces/Workflow_examples/latest/ and https://hub.knime.com/schroedinger/spaces/LiveDesign_models/latest/



New features in the KNIME extension

In Schrödinger Suite 2021-4

2021-4 New Features

- Includes the latest version of KNIME (v4.4.1)
- The Protein preparation workflow node uses the new Maestro panel
- Extra control on the Jaguar node calculations (eg atom constraints)

Run from LiveDesign:

- Upload workflows as protocols
- Protocol taking multiple columns as input

KNIME Analytics Platform 4.4 – some new features

KNIME analytics platform

- File handling
 - New connectors (including a Samba connector), updated nodes, and updates to the framework
- Conda environment propagation for R
- Snowflake in-Database processing
- New H2O autoML nodes

Some node improvements

- Variable creator
 - Specify a number of new flow variables at once
- Enhanced variables scopes
 - Variables defined or modified in loops, if-statements and try-catch are now accessible downstream

- REST nodes error handling
- Indexing and searching nodes

Newly moved out of Labs

- Joiner
- Integrated Deployment
 - Capture and write workflows for continuous and integrated deployment
 - New nodes, including the Workflow Reader and the Workflow Summary Extractor
- MongoDB, PowerBI

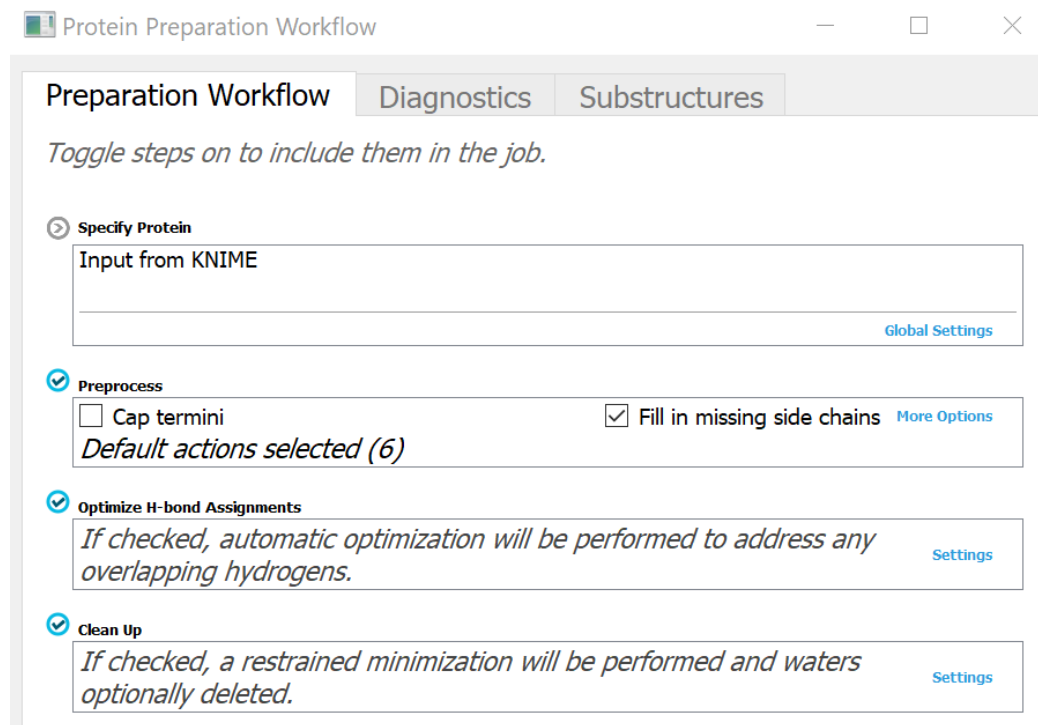
KNIME server

- Data Apps
 - Embedded Data Apps
 - Dynamic Data Apps
- Schedule retries for Server

See details in <https://www.knime.com/whats-new-in-knime-44>

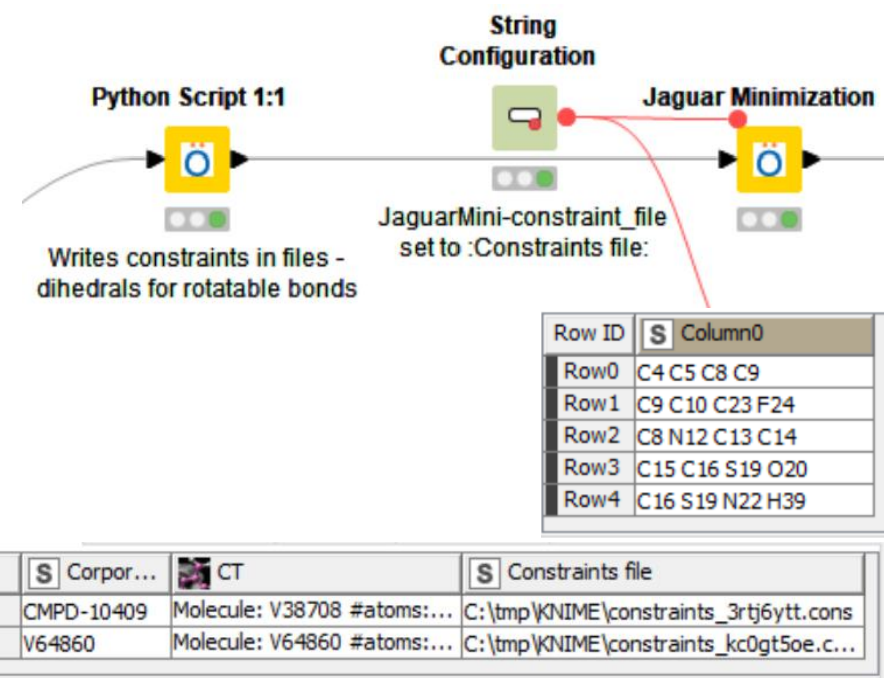
Protein preparation workflow node

- Configuration using the new Maestro panel
- In Labs for now and will replace the Protein preparation wizard node
 - To be replaced in existing workflows
 - Use the command reported in the variable tab to configure the new node



Jaguar and BLAST nodes

- Extended control on the Jaguar node calculations
 - Add an extra section to Jaguar calculation input
 - eg atom coordinate constraints
 - Using Parameter flow variable controls:
 - constraint_file <file>
 - or more generic: -add_section <file>
 - The content of the file is appended to the jaguar .in file
 - It was already possible to add and remove .in file keywords with Parameter flow variables

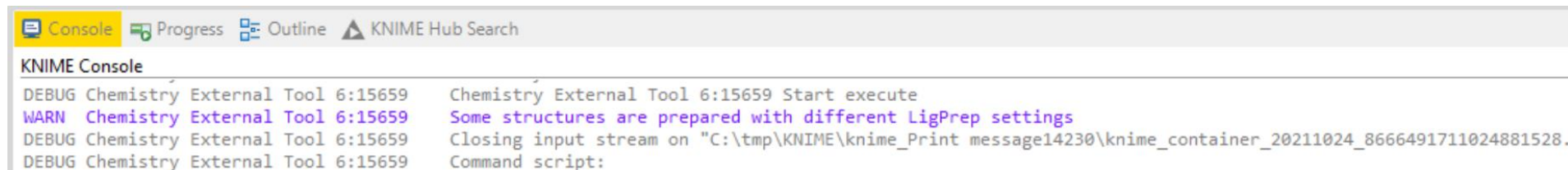
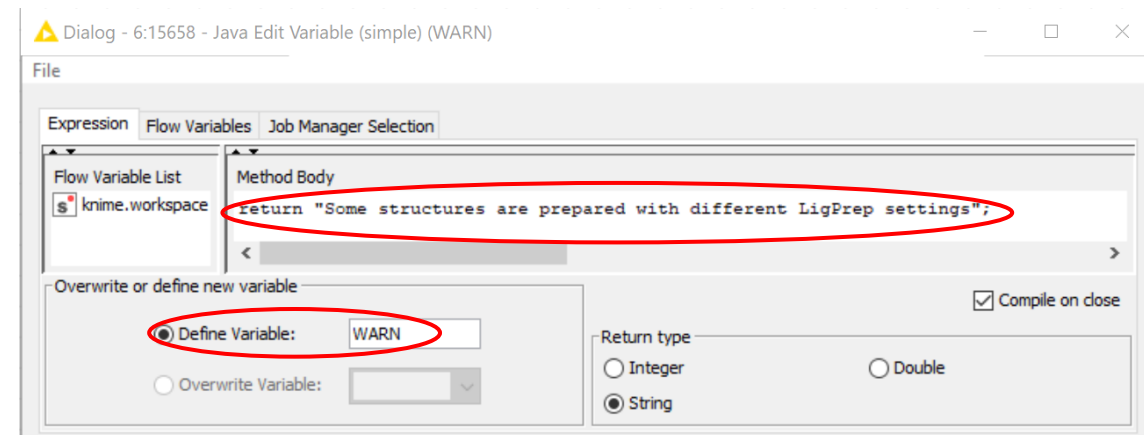
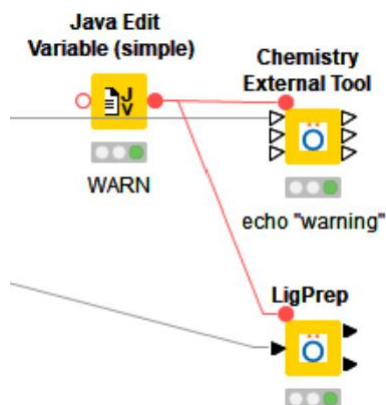


- Control where to run BLAST node search
 - Whether to run the BLAST search locally (downloaded or standard blast databases)
 - or remotely (via a web connection to NCBI)

The screenshot shows the configuration window for the BLAST node. It has tabs for 'BLAST', 'Job control', 'Flow Variables', 'Job Manager Selection', and 'Memory Policy'. The 'BLAST' tab is active, showing options for the input column, database (set to 'pdb'), location to run BLAST (with 'Remote' selected), and checkboxes for 'Filter query sequence' and 'Expand non-redundant hits'.

Batch execution – print message and testing

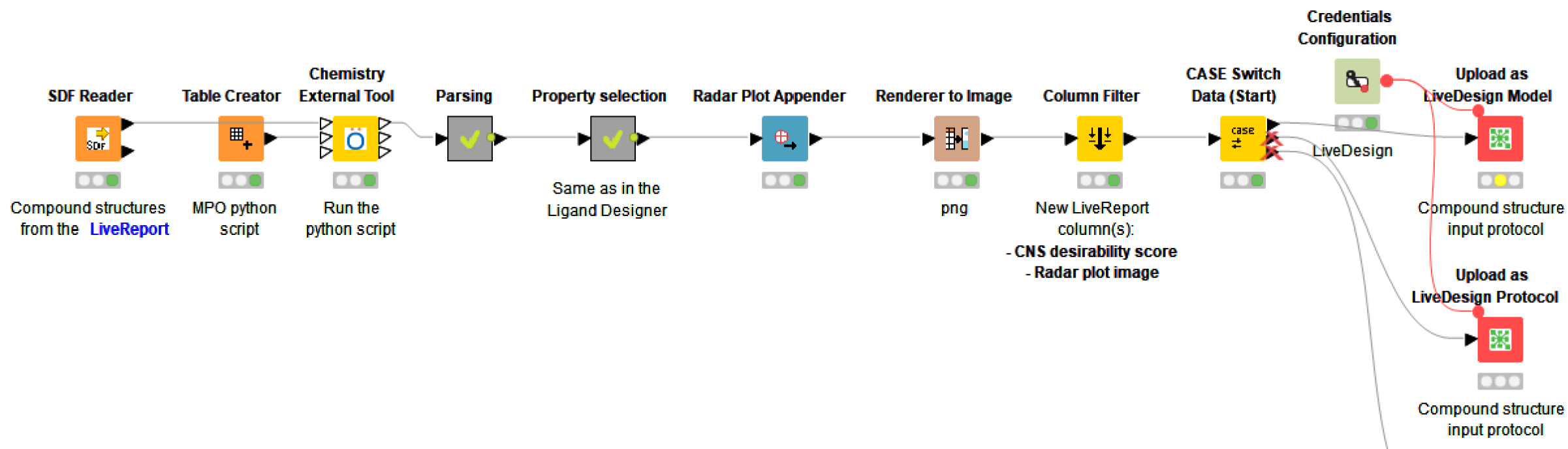
- Print messages in the console
 - User defined text printed
 - And verbosity level controlled with the variable name: DEBUG, INFO, WARN or ERROR
 - eg issue clear warning when running workflows in batch/in LiveDesign



- Batch test node
 - Existing arguments can be passed and are replaced in the workflow invocation
 - So diverse scenarios can be tested

Upload workflows to LiveDesign – 2 nodes

- Upload as model
 - Using one of the 3 generic KNIME protocols already deployed
- Upload as protocol
 - Using one of the protocol templates
 - Models created from the Admin page



Upload workflows as LiveDesign protocols

- Node
 - Configuration similar to the Upload as LiveDesign model node
 - Protocol templates available under `$SCHRODINGER/knime-v*/data/livedesign_protocols`
- Advantages
 - More user friendly Parametrize model panel
 - Dedicated field description
 - Value (the argument is included in the Protocol command)
 - Select the columns to display in the model among the predictions defined in the protocol (eg log column, query structure)
 - Output value aggregated or not:
each protocol can be listed on https://appsci-ld.onschrodinger.com/admin/ldproperties/ldproperty/UNAGGREGATED_MODEL_PROTOCOLS

Upload as LiveDesign Protocol | Flow Variables | Job Manager Selection

LiveDesign host: From the Preferences

Schrodinger Suite: From the Preferences

LiveDesign project: From the Preferences

Path to template protocol: protocols\KNIME_Compound_structure_template.zip

Corporate ID column: Corporate ID

3D column type: Ligands

Command type: Normal

☒ Overwrite Model

PyMOL script:

OK Apply Cancel ?

Upload workflows as LiveDesign protocols

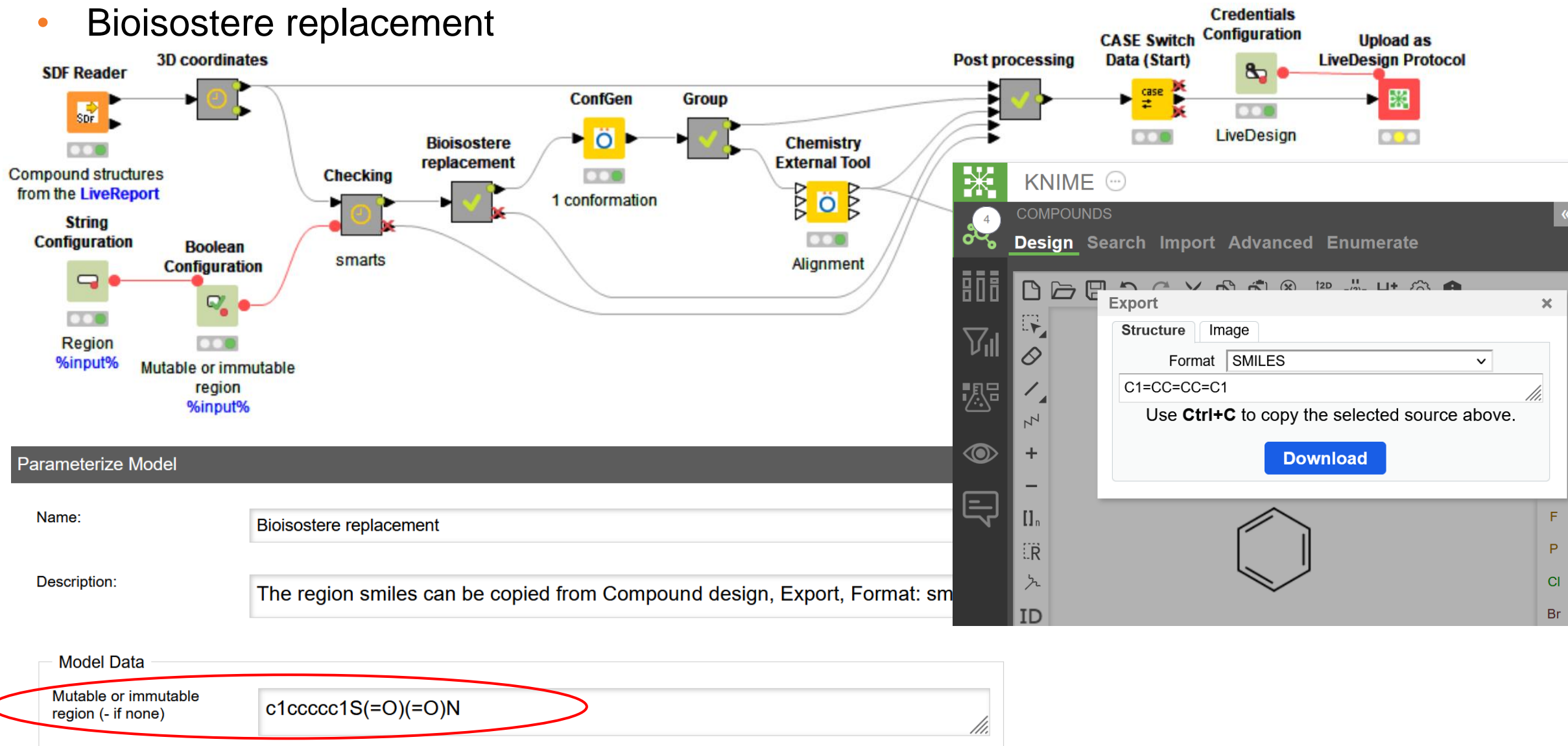
- **Models**
 - Created manually on the Admin page
 - Possibly system specific files or settings
 - Same philosophy as the other models (eg Glide docking)

| | KNIME workflows | Docking |
|-------------------------------|---|--|
| Protocol | Specific workflow | Glide settings (input file) |
| Model | Project or target specific files or settings (eg alignment template file) | Glide grid, Hbond constraints, core constraints... |
| Parametrized model (optional) | Settings changed at the time of the execution, input column selection... | Settings changed at the time of the execution |

- Alternative to using the generic KNIME protocols and the Upload workflows as LiveDesign model node
 - Model created in 1 step

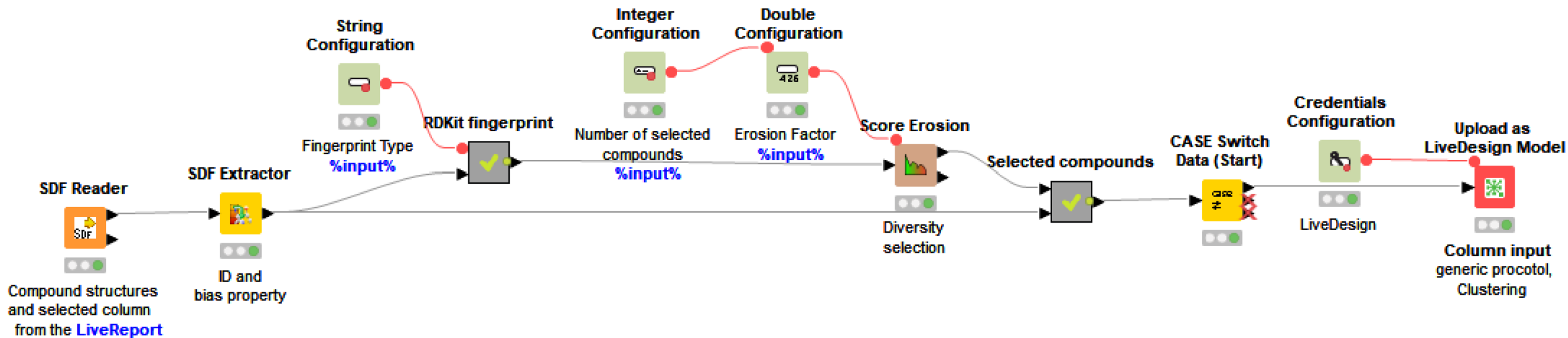
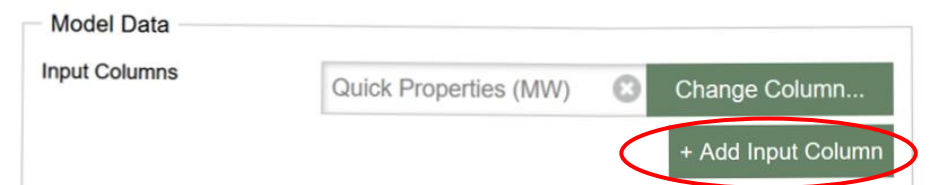
Upload as protocol – example

- Bioisostere replacement



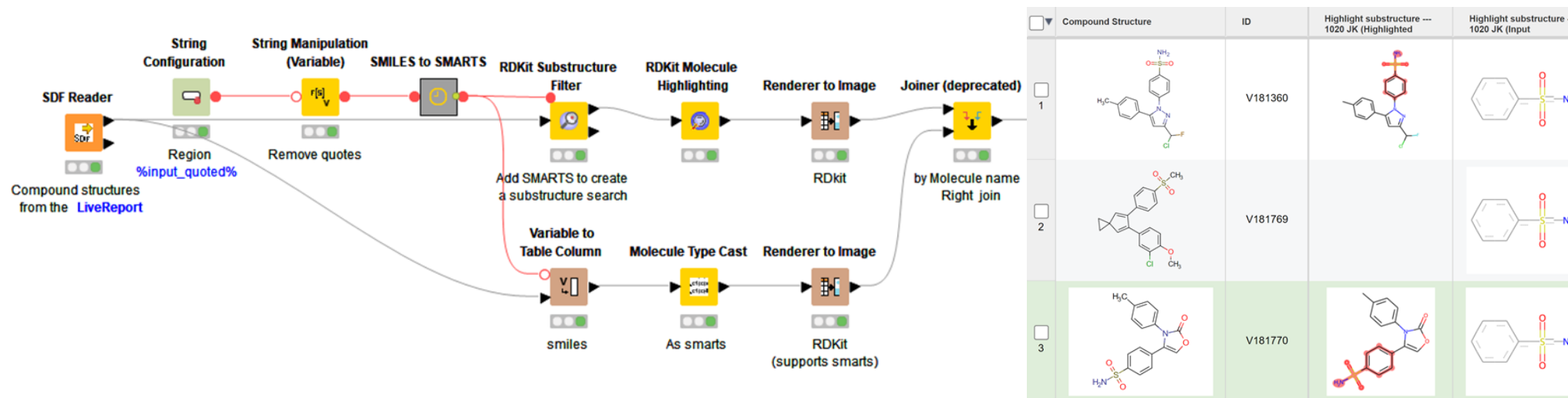
Protocol taking multiple columns as input

- New generic protocol taking:
 - One or several numeric or string columns (no 3D column for now) as input
 - And the compound structures
- The input is a SD file with the column values as properties
- Application example:
Biased diversity selection
 - Among the compound structures in the LiveReport
 - And biased based on a user specified column



Workflow examples and validated LiveDesign models

- Protein – Descriptors: Protein descriptors calculated based on the sequence or the 3D structure
- LiveDesign model – Cheminformatics – Biased diversity selection using the score erosion algorithm to select a subset of compounds that have the highest value in the selected column and as diverse as possible.
- LiveDesign model – Cheminformatics – Highlight substructure



Available on: https://hub.knime.com/schroedinger/spaces/Workflow_examples/latest/ and https://hub.knime.com/schroedinger/spaces/LiveDesign_models/latest/



New features in the KNIME extension

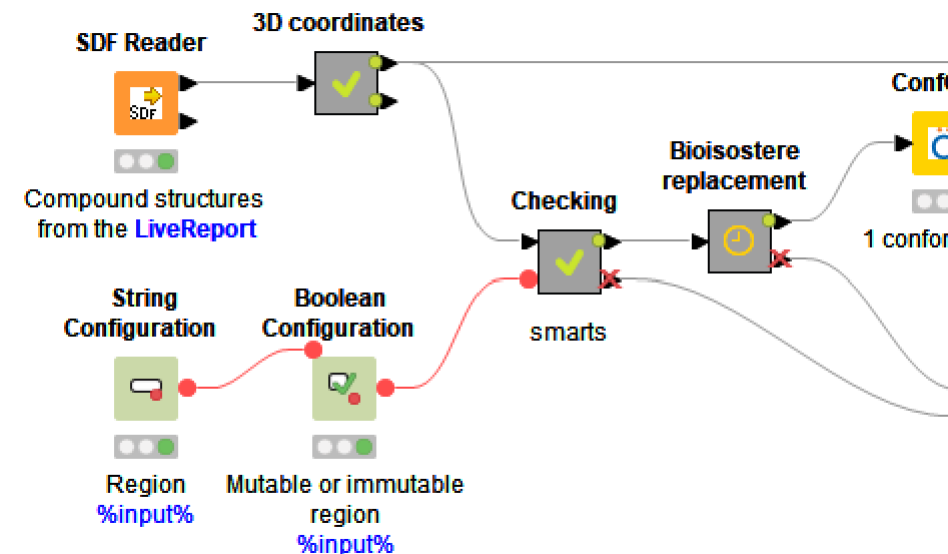
In Schrödinger Suite 2021-3

KNIME in LiveDesign:

- Upload as LiveDesign model node
 - The extra argument and extra file fields are populated automatically
 - The model folder can be set in the Preferences
- Model administration
 - A new node lists the protocols and models deployed on a LiveDesign host
 - Models can be archived using LiveDesign_admin.py script

Upload as LiveDesign model – extra argument and extra file fields

- The extra argument and extra file fields are populated automatically
 - For the nodes tagged with *%input%*
 - Find the list of supported nodes in the output of the Get help node with `$SCHRODINGER/run KNIME_batch.py` and `-print_allowed`
 - In a Parametrized model the CSV reader node taking the data from the LiveReport must be tagged with *LiveReport*
- These fields can be exposed in the Parametrize model panel
 - Changing the Parameter source on the model Admin page



| MODEL DATA | | | |
|--------------------------|----------------|--|------------------|
| NAME | PARAMETER TYPE | DATA ⓘ | PARAMETER SOURCE |
| extra argument 1 (20927) | | | |
| extra argument 1 | Text | Parent Data: -dummy -region 'c1cccc1' | Set Default ▾ |
| extra argument 2 (20942) | | | |
| extra argument 2 | Text | Parent Data: -dummy -mutable false | Set Fixed ▾ |
| extra argument 3 (20924) | | | |
| extra argument 3 | Text | Parent Data: -dummy -dummy | Set Fixed ▾ |

Upload as LiveDesign model – protocols

- Protocol simplification
 - The extra argument and extra file fields are at the top of the model Admin page
 - Followed by the other editable fields
 - The hard coded fields are at the bottom
 - Simplified command sections:

```
COMMAND
ID 1996
# Preprocessing
export SCHRODINGER=${SCHRODINGER:TEXT-INPUT}
export PYMOL_EXEC=${PYMOL_EXEC:TEXT-INPUT}

# Unzip the required utilities
unzip $(Zipped utilities:FILE-INPUT)
bash $PWD/check_environments.sh

# Add the livereport columns as properties to the Compound structure
$$SCHRODINGER/run $PWD/multicolumn_to_sdf.py -input $(SDF-FILE) -multicolumns $(Input Columns:MULTI-COLUMN-INPUT) -output added_columns.sdf

$$SCHRODINGER/run $PWD/preprocess_protocol.py -extra_arg_1=${extra argument 1:TEXT-INPUT} -extra_arg_2=${extra argument 2:TEXT-INPUT} -extra_arg_3=${extra argument 3:TEXT-INPUT} -extra_file_1=${extra file 1:FILE-INPUT} -extra_file_2=${extra file 2:FILE-INPUT} -extra_file_3=${extra file 3:FILE-INPUT}

touch $(workflow svg file:FILE-INPUT)
ls $$SCHRODINGER/knime-v*/data/*UpdateSite*

ID 1997
# Install extra KNIME extensions
export SCHRODINGER=${SCHRODINGER:TEXT-INPUT}

$$SCHRODINGER/run $PWD/KNIME_install.py -features_list $(extra extensions:FILE-INPUT) -verbose -keeplogs -configuration $PWD/ExtraExtensions /configuration $$SCHRODINGER/knime-v*/bin/Linux-x86_64/knime

ID 1998
# KNIME batch execution
$(Queue eg #te_queue=knime or echo "default queue":TEXT-INPUT)
export PYMOL_EXEC=${PYMOL_EXEC:TEXT-INPUT}
export SCHRODINGER=${SCHRODINGER:TEXT-INPUT}
export SCHRODINGER_FEATURE_FLAGS=${JOB_SERVER}

$$SCHRODINGER/run $PWD/KNIME_batch.py $(workflow:FILE-INPUT) -run -sdf added_columns.sdf -stderr $(KNIME logs verbosity:TEXT-INPUT) -deleteTempFiles false -schrodingerTempDir $PWD -knimeTempDir $PWD -destFile=$PWD/Executed.knwf $(Extra options eg -force_newer:TEXT-INPUT) $(extra argument 1:TEXT-INPUT) $(extra argument 2:TEXT-INPUT) $(extra argument 3:TEXT-INPUT) $(extra argument 4:TEXT-INPUT) $(extra argument 5:TEXT-INPUT) $(extra argument 6:TEXT-INPUT) -data workspace -configuration $PWD/ExtraExtensions/configuration -HOST $(KNIME Primary host:TEXT-INPUT)

ID 1999
# Post-processing
export SCHRODINGER=${SCHRODINGER:TEXT-INPUT}

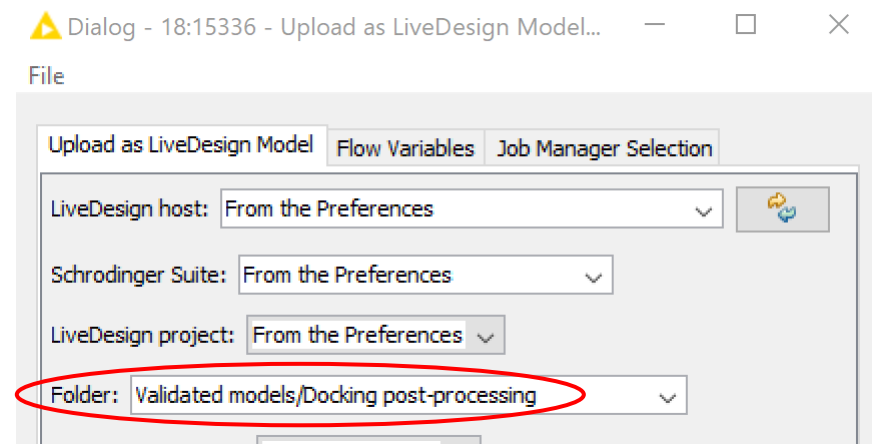
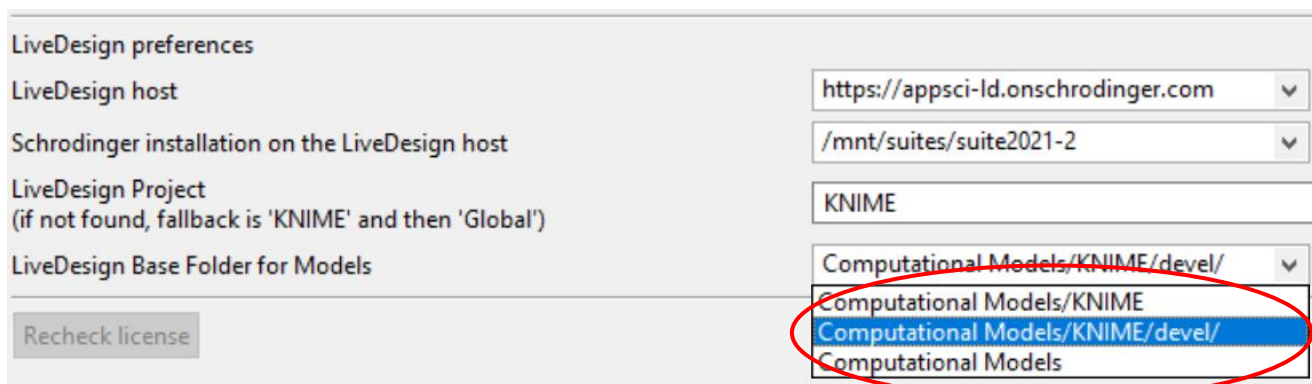
$$SCHRODINGER/run $PWD/postprocess_results.py > postprocess.log 2>&1
cat $PWD/$(results.csv or - to investigate temporary files:TEXT-INPUT)
```

| | | |
|--|------|---|
| Extra options eg -force_newer (21161) | Text | Parent Data: <i>-debug</i> <input type="text" value="-debug"/> |
| KNIME logs verbosity (21166) | Text | Parent Data: <i>INFO</i> <input type="text" value="INFO"/> |
| KNIME Primary host (21169) | Text | Parent Data: <i>localhost:1</i> <input type="text" value="localhost:1"/> |
| PYMOL_EXEC (21158) | Text | Parent Data: <i>/mnt/pymol/pymol</i> |
| Queue eg #te_queue=knime or echo "default queue" (21157) | Text | Parent Data: <i>echo "default queue"</i> <input default="" queue\""="" type="text" value="echo \"/> |
| results.csv or - to investigate temporary files (21167) | Text | Parent Data: <i>results.csv</i> <input type="text" value="results.csv"/> |
| SCHRODINGER (21163) | Text | Parent Data: <i>/mnt/suites/suite2021-3</i> <input type="text" value="/mnt/suites/suite2021-3-ob-latest"/> |

| | | |
|---------------------------|------|---|
| workflow (21160) | File | Currently: <i>Computational Models/KNIME/devel/Valid with a pharmacophore.knwf</i> <input type="checkbox"/> Clear Change: <input type="button" value="Browse..."/> No file selected. |
| workflow svg file (21155) | File | Currently: <i>workflow.svg</i> <input type="checkbox"/> Clear Change: <input type="button" value="Browse..."/> No file selected. |
| Zipped utilities (21168) | File | Parent File: <i>utilities.zip</i> |

Upload as LiveDesign model – model folder

- The model folder can be set in the Preferences
 - To deploy several copies of a model in various folders
 - Without changing the workflow name
 - Possibly combined with a subfolder specified in the Upload node Folder field
 - It helps organizing the models, collaborating with colleagues...



- Usage examples:
 - The production version of the models can be deployed and organized in:
Computational Models/Cheminformatics /Docking /ADME ...
 - The versions under development deployed under: Computational Models/KNIME/Development/
 - The versions to test (eg modified by a colleague) under: Computational Models/Tests/

Model administration – list models and protocols

- List LiveDesign items node

- Lists the protocols or models for a specified parent
 - Or all the protocols deployed if no parent ID is provided
- Optional filter by name in the Extra arguments field
- The Admin page information and more (projects the model is deployed to) are also reported
- Usage examples:
 - Check the deployed protocols and models and move some to other folders or projects
 - List the parametrized models created for a model

Dialog - 10:16151 - List LiveDesign Items (KNI... — □ ×

File

List LiveDesign Items Flow Variables Job Manager Selection Memory Policy

LiveDesign host:

Column containing Parent id:

Extra arguments:

OK Apply Cancel ?

| Row ID | <input type="checkbox"/> Name | <input type="checkbox"/> Id | Txt Description | <input type="checkbox"/> Folder | <input type="checkbox"/> Parent | <input type="checkbox"/> User | <input type="checkbox"/> Projects |
|--------|-------------------------------|-----------------------------|--|---|---------------------------------|-------------------------------|-----------------------------------|
| Row2 | ADME | 2138 | 2021/06/29 17:41:03 --- ADME : Calculates ADME properties with QikProp. | Computational Models/KNIME/devel/Validated models/ADME and molecular properties | 2061 | jonas.k... | KNIME |
| Row3 | Atropisomerism | 2139 | 2021/06/29 17:33:31 --- Atropisomerism : It detects atropisomers in input structures. Each rotata... | Computational Models/KNIME/devel/Validated models/ADME and molecular properties | 2061 | jonas.k... | KNIME |
| | | | 2021/06/30 10:09:44 | | | | |

Model administration

- Archive models
 - Using LiveDesign_admin.py

```
"$SCHRODINGER"/run -FROM knime LiveDesign_admin.py -type model -mode archive -host <LiveDesign host> -id <model ID> -username <username>
```
 - Applicable to any model (not only the KNIME ones)
- Option to control the model Command type
 - In LiveDesign_admin.py command and in the LiveDesign upload models node in the Extra arguments field
 - eg -command_type CLICK_TO_RUN

Dialog - 19:15913 - Upload LiveDesign Models (On the same host,) — □ ×

File

Upload LiveDesign Models | Flow Variables | Job Manager Selection | Memory Policy

LiveDesign host:

Column containing model filepath::

Column containing New name (optional):

LiveDesign Protocol:

Column containing folder name

Default Folder:

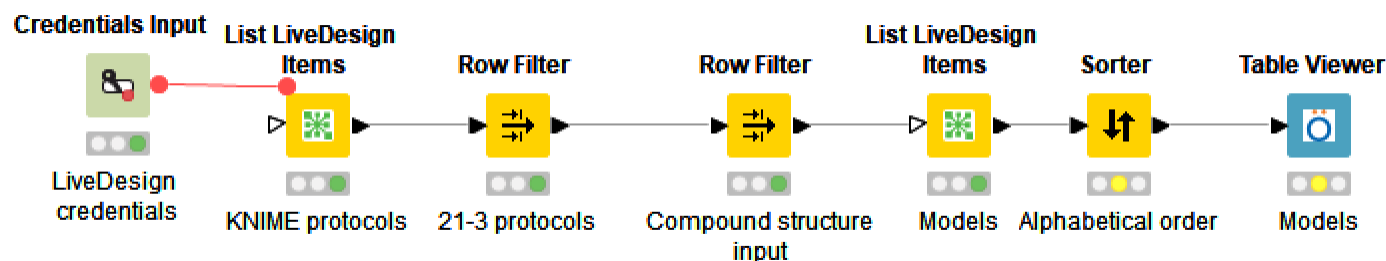
Projects:

Schrodinger Suite:

Extra arguments:

Components and Workflow Examples

- LiveDesign - Administration - List models and protocols



Improved LiveDesign models:

- Low energy conformations
- Ligand alignment with a pharmacophore

Available on: https://hub.knime.com/schroedinger/spaces/Workflow_examples/latest/ and https://hub.knime.com/schroedinger/spaces/LiveDesign_models/latest/



New features in the KNIME extension

In Schrödinger Suite 2021-2

2021-2 New Features

- Includes the latest version of KNIME (v4.3.2)
- New **Ligand alignment** node

KNIME in LiveDesign:

- Generic protocols
 - More **arguments fields** to control the workflow
 - Control the computationally expensive calculation distribution
- Upload as LD model node
 - By default in the **project** that is set **in the Preferences**
 - A surface can be added to a receptor-ligand complex column
 - The models can also be uploaded from Maestro
- New **LiveDesign connection** node used as input for the Import and export to LiveDesign nodes

KNIME Analytics Platform 4.3 – some new features

KNIME Analytics Platform

- File Handling Framework
- Improved Reader & Writer nodes
- Columnar table backend for fast tables
- Python enhancements
- More Utility Nodes
 - Variable to Credentials, Table Manipulator
- Components
 - Building Components - Dialog Layout

KNIME Hub

- Flexibility in Creating Spaces
 - Create, rename, and delete your spaces from the browser

- Collaborate: work together on public spaces

- KNIME Analytics Platform Integration

KNIME Server

- Monitoring Portal
- RabbitMQ for High Availability
- KNIME Server Large and Executors on Azure

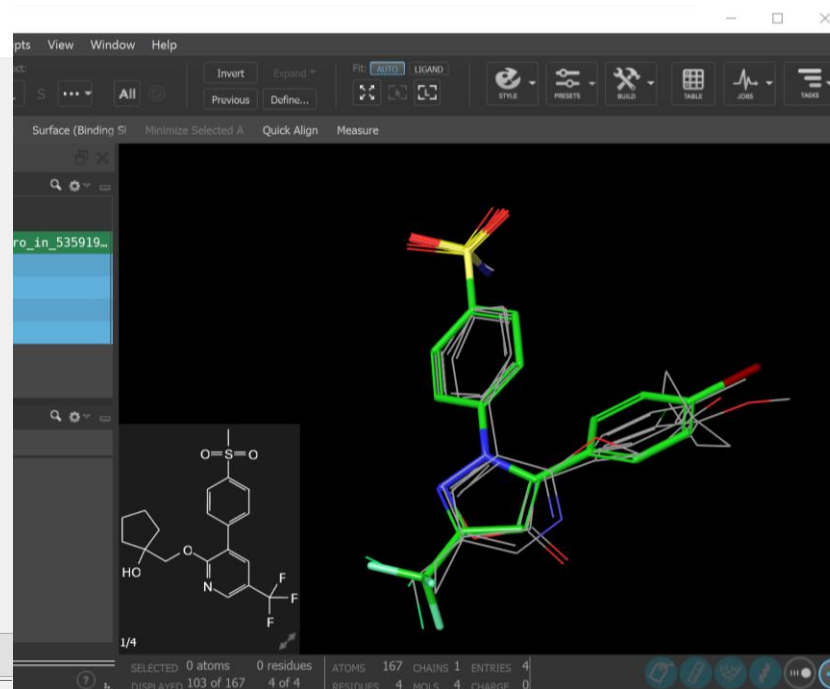
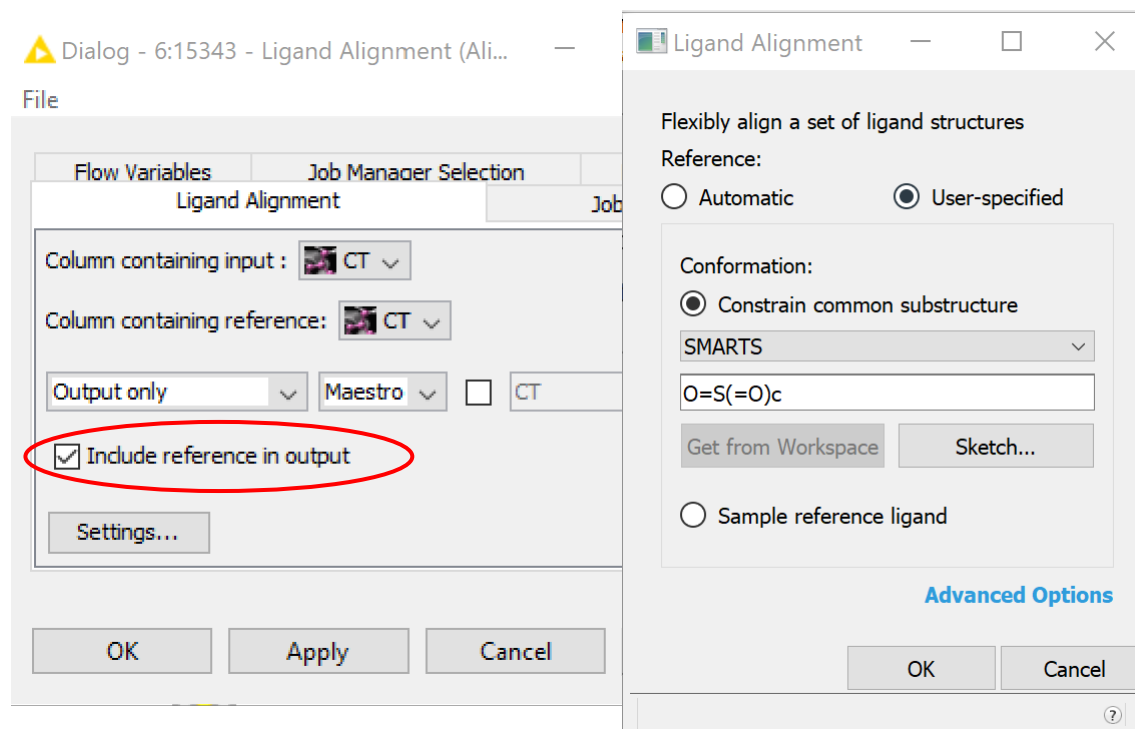
Community and Partner Extensions

- Chemaxon/Infocom Marvin Extensions, H2O Driverless AI, Redfield BERT

See details in <https://www.knime.com/whats-new-in-knime-43>

Ligand alignment node

- Various alignment methods
 - Align congeneric or non-congeneric ligands
 - Optional input port for the reference structure
- Using the same configuration panel as Maestro



KNIME LiveDesign generic protocols

- Up to 6 extra argument fields
 - to control more workflow steps from the Admin page or the Parametrize model panel
 - 3 first ones can be used for file selection
- Schrodinger version independent
 - eg keep using an old Schrodinger version to have consistent results in a project

| | | |
|--------------------------|------|---|
| extra argument 1 (15217) | Text | Parent Data: <i>-dummy</i> -LigPrep_options "-s4 -pht 2" |
| extra argument 2 (15222) | Text | Parent Data: <i>-dummy</i> -igrid MySystem.zip |
| extra argument 3 (15233) | Text | Parent Data: <i>-dummy</i> -alignment_ref core.mae |
| extra argument 4 (15240) | Text | Parent Data: <i>-dummy</i> -alignment onFile |
| extra argument 5 (15220) | Text | Parent Data: <i>-dummy</i> -POSES_PER_LIG 5 |
| extra file 1 (15238) | File | Parent File: <i>mockup.txt</i> Currently: <i>mockup.txt</i> <input type="checkbox"/> Clear Change: <input type="button" value="Browse..."/> No file selected. |
| extra file 2 (15231) | File | Parent File: <i>mockup.txt</i> Currently: <i>mockup.txt</i> <input type="checkbox"/> Clear Change: <input type="button" value="Browse..."/> grid_1bl7.zip |
| extra file 3 (15223) | File | Parent File: <i>mockup.txt</i> Currently: <i>mockup.txt</i> <input type="checkbox"/> Clear Change: <input type="button" value="Browse..."/> core.mae |

KNIME LiveDesign generic protocols

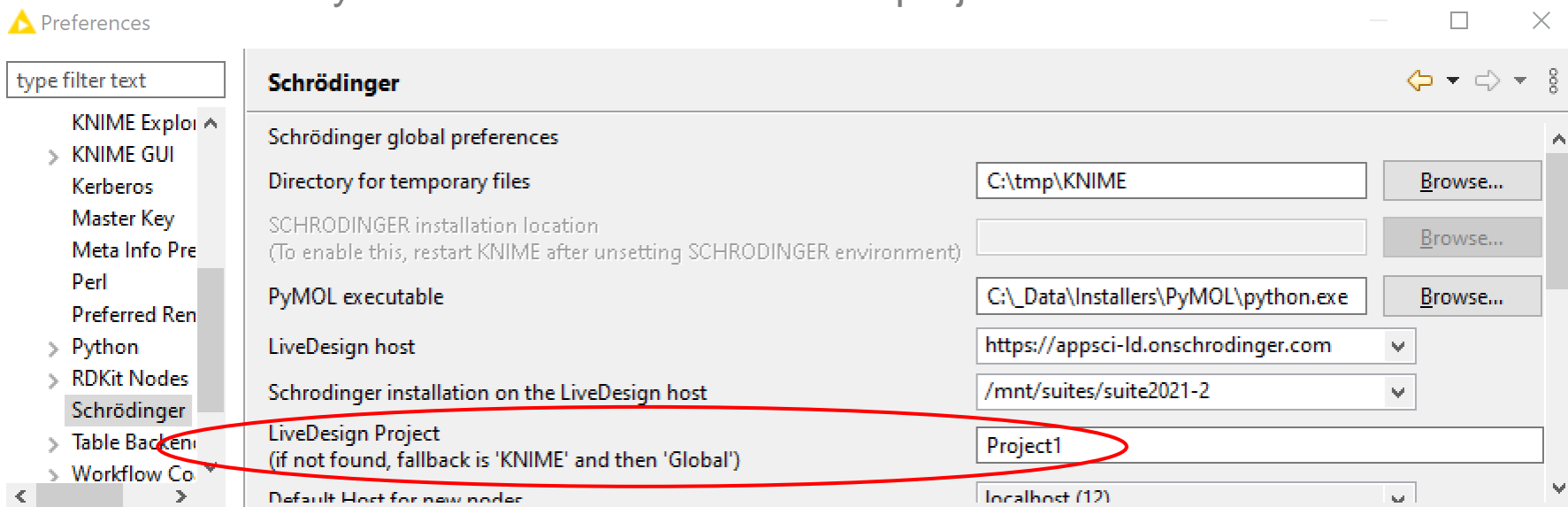
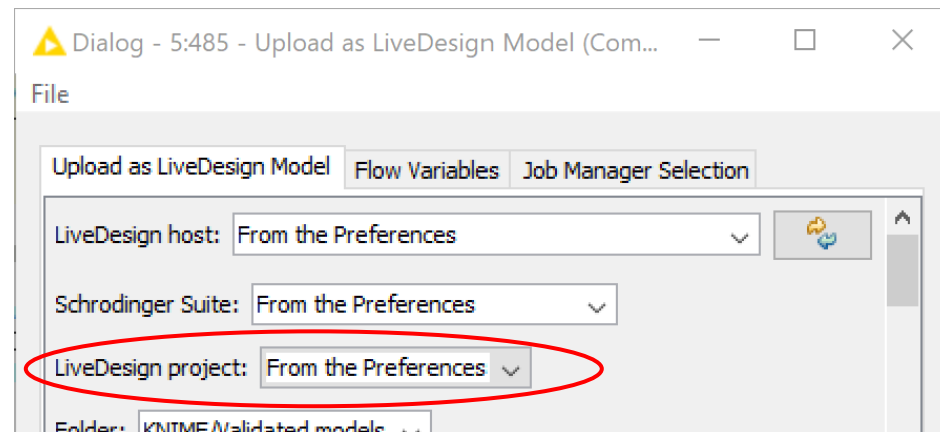
- Schrodinger and PyMOL installation paths
 - Clearer error message when they aren't valid
 - List the installations in the directory
 - Check if there is a newer installation available
- Control over job distribution
 - Set the machine and number of CPUs to use
 - For the computationally intensive calculations with Schrodinger nodes
 - LiveDesign machine and 1 CPU by default

Standard Out:

```
SCHRODINGER installation is not available at /mnt/suites/suite2021-2
Available SCHRODINGER installations at /mnt/suites
=====
suite2021-1
suite2021-1-nb148
suite2021-1-ob123
suite2021-1-ob140
suite2021-1-ob156
suite2021-1.RDKit_2020_09_5
suite2021-2-nb077
suite2021-2-nb086
```

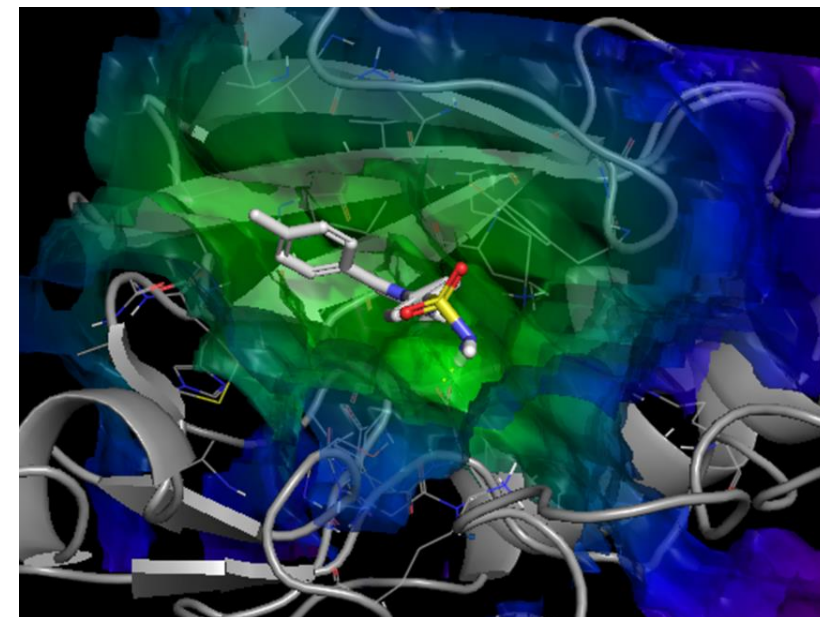
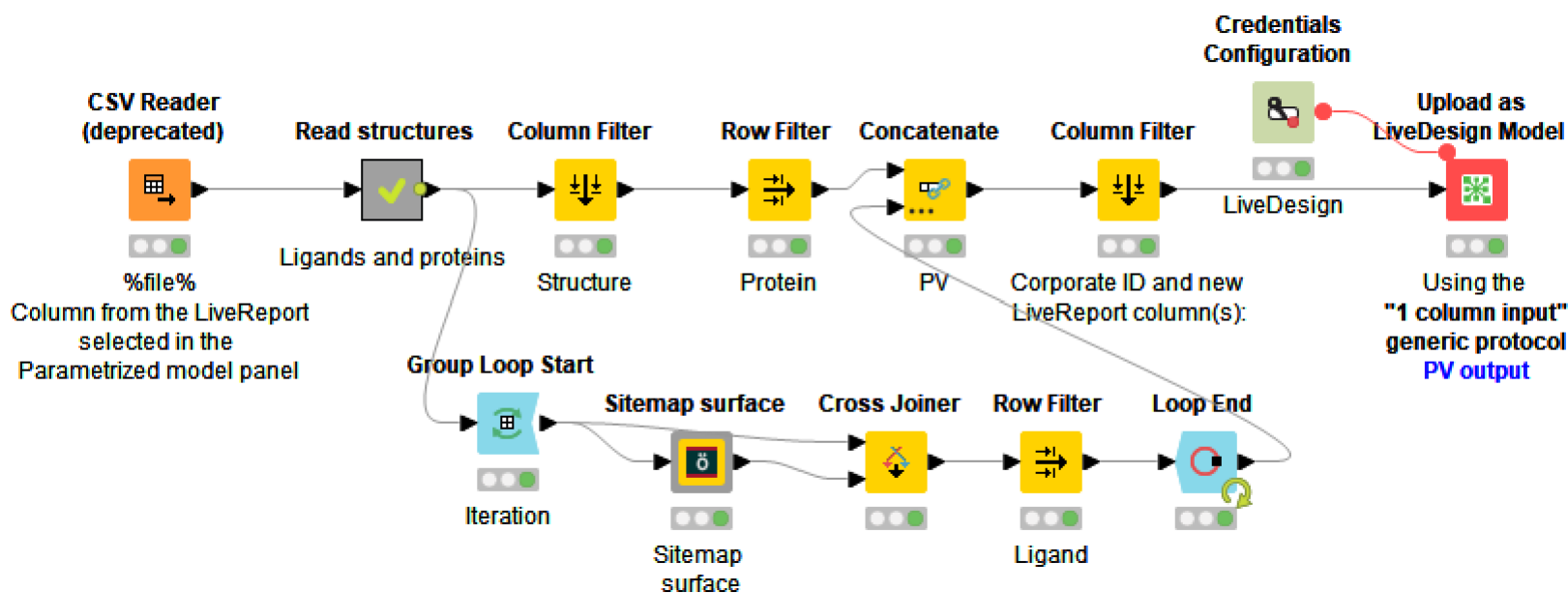

Upload as LiveDesign models node

- Create Project specific KNIME Models
 - Project set in the Preferences the Project
 - To create models in a specific project by default instead of making them available globally
 - To be set to a personal or a testing project
 - Project1 by default and fallback to KNIME and global
 - And changed to a specific target project in the node
 - It helps keeping the Data & Columns tree clear
 - Only the relevant models in each project



Upload as LiveDesign models node

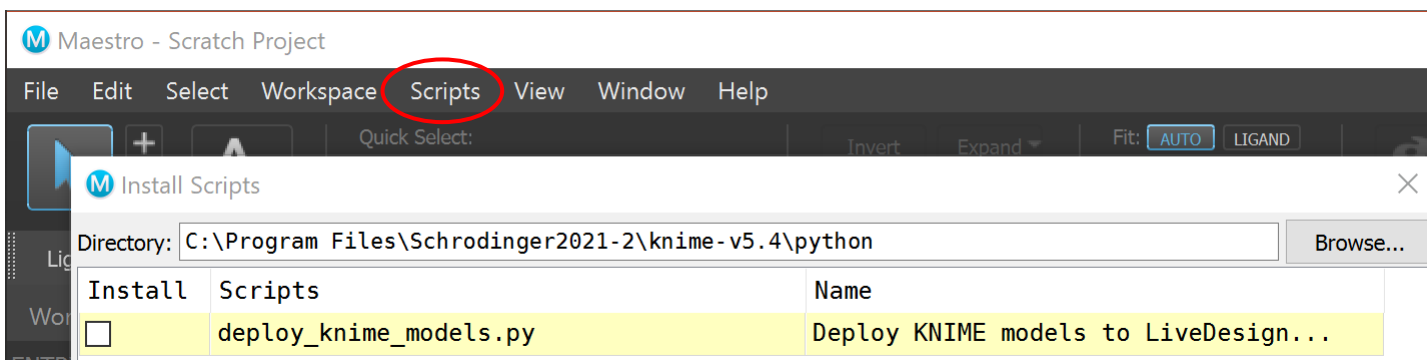
- Surface for receptor-ligand complexes
 - Already for ligands and docked poses
 - eg Binding pocket surface model
- from a receptor-ligand complex column in the LiveReport



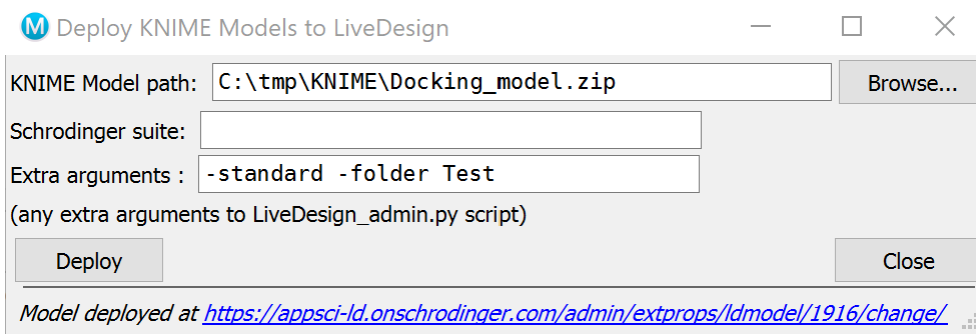
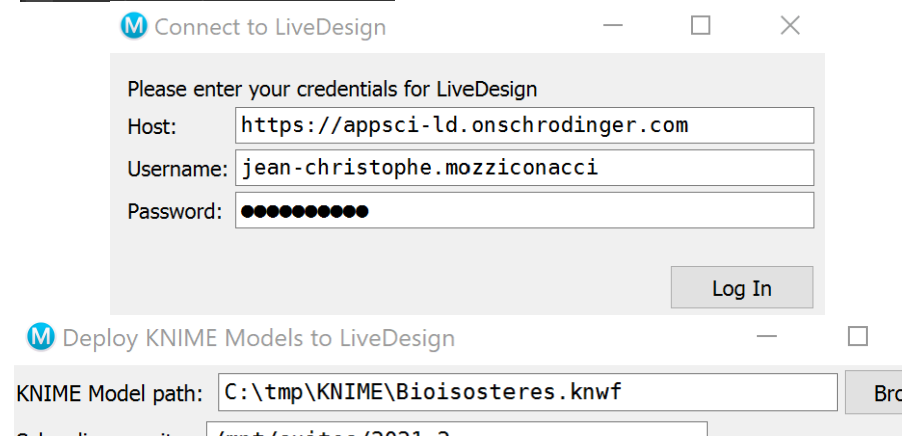
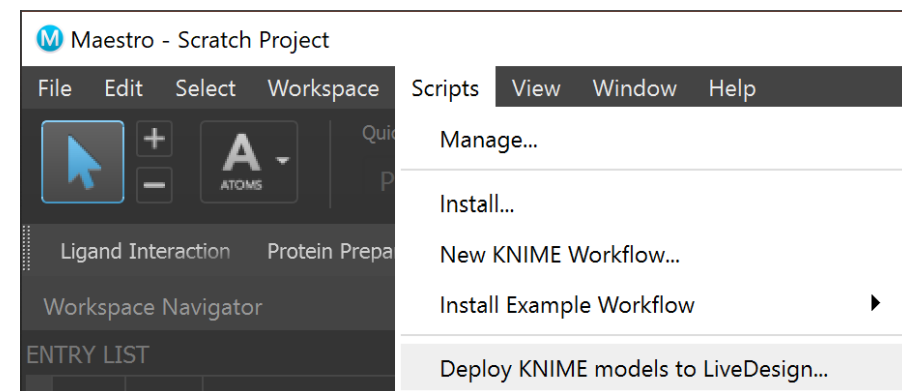
Model upload

- Script in Maestro

- Available to be installed in Maestro:
`$SCHRODINGER/knime-v*/python/deploy_knime_models.py`

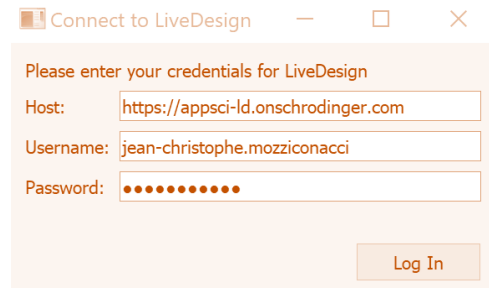


- Interface of choice for the modelers
Alternative to the KNIME upload node, administration node and LiveDesign_admin.py script
- Upload any LiveDesign model (not only KNIME based ones)



LiveDesign Connection node

- Connection information required
 - The Credential input connector node can still be used
- All the configuration information
 - Including the host name
 - Better integration with the Maestro panels



Connect to LiveDesign

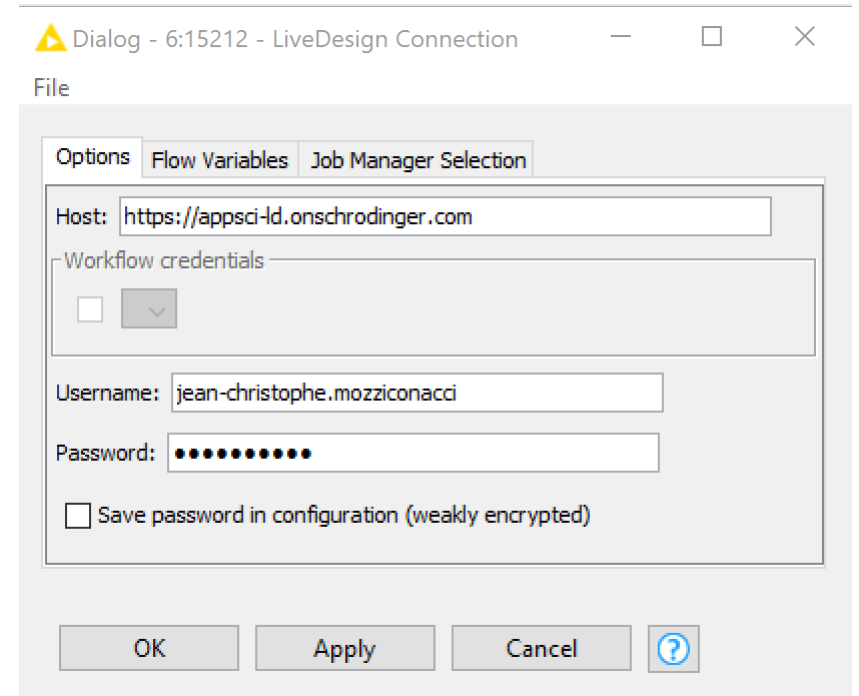
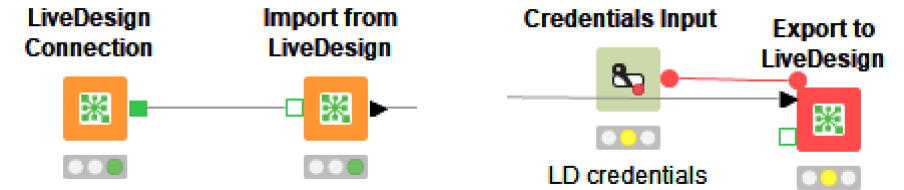
Please enter your credentials for LiveDesign

Host:

Username:

Password:

- Supported by the Import and export to LiveDesign nodes for now



Dialog - 6:15212 - LiveDesign Connection

File

Options | Flow Variables | Job Manager Selection

Host:

Workflow credentials

☐

Username:

Password:

☐ Save password in configuration (weakly encrypted)

Workflow Examples and LiveDesign models

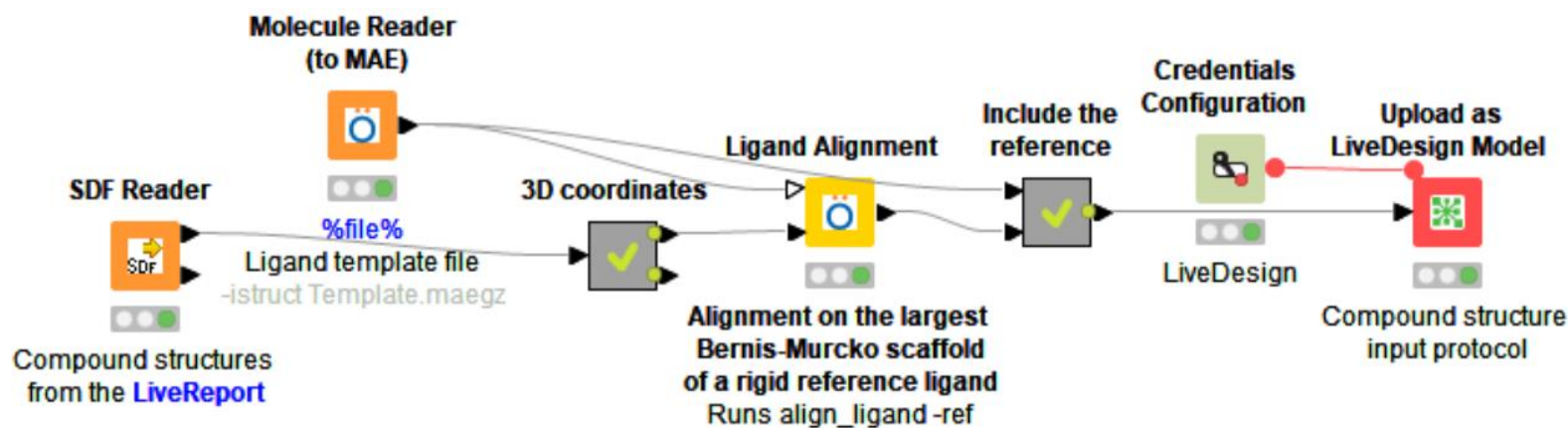
- General – Ligand alignment : new node usage
- Import and export from LiveDesign : uses LiveDesign Connection node

New LiveDesign model:

- Interaction surface
 - from a receptor-ligand complex column in the LiveReport

Improved LiveDesign models:

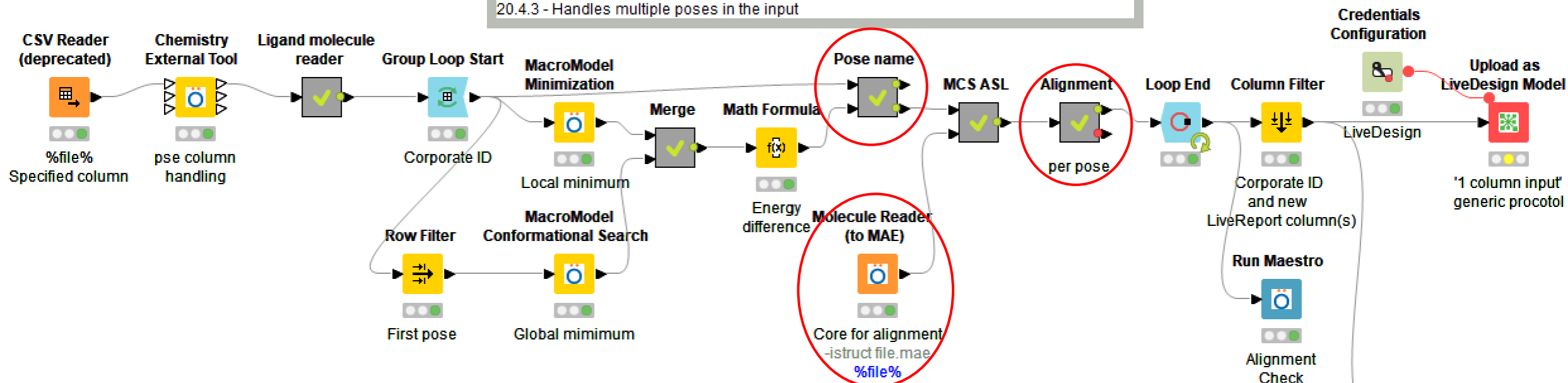
- Structure alignment – Ligand alignment with a cocrystallized reference : Using the new Ligand alignment node



Workflow Examples and LiveDesign models

- Low energy conformations
 - Control to generate several LigPrep forms
 - Alignment on a reference ligand (or a core section) specified on the admin page
 - Using MacroModel or ConfGen
- Binding pose strain

Changelog:
21.1.3 - Pose reordering
Alignment on each binding pose
Optional alignment on a specified section of the ligands
21.1.2 - More robust energy difference calculation
21.1.1 - Energy difference in kcal/mol
20.4.3 - Handles multiple poses in the input





New features in the KNIME extension

In Schrödinger Suite 2021-1

KNIME in LiveDesign

- Free file name choice in the **Extra file fields** and other usability improvements in the 2 generic protocols
- The **model the description** is updated from the workflow when deployed and the models can be sorted by modification date on the admin page
- New LiveDesign model and protocol **administration nodes**, running the script LiveDesign_admin.py
- Supports the latest version of KNIME (v4.3, but includes v4.1.3)
- Include the biological unit and set the source in the Get PDB node
- The Jaguar minimization node runs on multiple CPUs

Generic protocols – extra file names

- Free file name choice in the Extra file fields
 - The files are renamed behind the scene to match the Extra argument corresponding field
 - System specific name recorded in the Column details
- Additional input configuration nodes supported
 - Table Reader and Writer
 - Boolean and List Box Configuration
 - The Credential configuration node can also be controlled using a Workflow credential
 - *Store your password as environment variable*
 - *Define a 'Workflow Credentials' variable*
 - *Set the KNIME server connection to get the credentials from this variable*
 - *`$SCHRODINGER/KNIME_batch.py - credential="credentials;<username>;$PASSWORD"`*

| | | |
|------------------|------|--|
| extra file 3 | File | Parent File: <i>mockup.txt</i> Currently: <i>reference.pdb</i> <input type="checkbox"/> Clear Change: <input type="button" value="Browse..."/> No file selected. |
| extra argument 3 | Text | <input type="text" value="-ipdb reference.pdb"/> |

Column Details

| Name | Data |
|------------------|--|
| extra argument 1 | -source PDB -preparationORnot preparation -minimizationORnot not |
| extra argument 2 | -reference File |
| extra argument 3 | -ipdb reference.pdb |
| extra file 1 | mockup.txt |
| extra file 2 | mockup.txt |
| extra file 3 | 1CX2 with V49629 docked with constraints.pdb |

Options | Flow Variables | Job Manager Selection | Memory Policy

KNIME Server:

Authentication: ☒ Credentials

☐ My KNIME server

☐ Server_credentials

☐ Id_credentials

Timeout (ms):

Generic protocols – improvements

- Reorganized in 4 sections for better readability
- New "extra extensions" field
 - For workflows including nodes from extensions not included in the default installation
 - Specify a file listing the extensions to install
eg `com.vernalis.knime.source.feature.feature.group`
`org.erlwood.features.cheminformatics.base.feature.group`
- Keep the temporary files for inspection
 - Especially useful to inspect the partially executed workflow to find which node(s) failed
 - "results.csv or - to investigate temporary files" field to get the task to fail
- More functionalities but still only 2 generic protocols:
 - KNIME Workflow - Compound structure input
 - KNIME Workflow - 1 column inputAvailable from `$SCHRODINGER/knime-v*/data/livedesign_protocols`

COMMAND

ID 7308

```
# Preprocessing
export SCHRODINGER=${SCHRODINGER:TEXT-INPUT}
${SCHRODINGER}/run ${Protocol Preprocess Script:FILE-INPUT}
-extra_arg_1="${extra argument 1:TEXT-INPUT}" -extra_arg_2="${extra
argument 2:TEXT-INPUT}" -extra_arg_3="${extra argument 3:TEXT-
INPUT}" -extra_file_1="${extra file 1:FILE-INPUT}" -extra_file_2="${extra
```

ID 7309

```
# Install extra KNIME extensions
export SCHRODINGER=${SCHRODINGER:TEXT-INPUT}
${SCHRODINGER}/run -FROM knime KNIME_install.py -features_list
${extra_extensions:FILE-INPUT} -verbose -keeplogs -configuration
$PWD/ExtraExtensions/configuration ${SCHRODINGER}/knime-v*/bin
/! linux-x86_64/knime
```

ID 7310

```
# KNIME batch execution
${Queue eg #te_queue=knime or echo "default queue":TEXT-INPUT}
export PYMOL_EXEC=${PYMOL_EXEC:TEXT-INPUT}
export SCHRODINGER=${SCHRODINGER:TEXT-INPUT}
${SCHRODINGER}/run KNIME_batch.py ${workflow:FILE-INPUT} -run -itxt
${Input column (see the model description):COLUMN-INPUT} -stderr
```

ID 7311

```
# Post-processing
cat $PWD/${results.csv or - to investigate temporary files:TEXT-INPUT}
```

Upload as LiveDesign model – model description and time stamp

- The model description is updated from the workflow description
 - Along with the tags and author
- It includes a modification time stamp
 - Latest updated models by sorting by Description on LiveDesign Admin page

Node Repository | **Description** | Workflow Coach | KNIME Hub Search

Binding pose strain

Title Binding pose strain

Description
Input: Select in the LiveReport a pose viewer 3D column from a
The model minimizes the binding pose conformation to a local search to find the global minimum.
Calculates the conformation energy difference between the local and the global minima
Aligns the global minimum conformation on the initial binding pose.
Output: The initial binding pose is the second pose in the 3D column and displayed without hydrogen.

Tags
LiveDesign MacroModel

Links
No links have been added yet.

Creation Date 2020-11-24

Author Schrodinger 20.4.3

Binding pose strain
Modified January 7, 2021 by jcmozzic
2021/01/07 15:18:07
--- Binding pose strain :
Input: Select in the LiveReport a pose viewer 3D column from a docking.
The model minimizes the binding pose conformation to a local minimum and runs a conformational search to find the global minimum.
Calculates the conformation energy difference between the local and the global minima
Aligns the global minimum conformation on the initial binding pose.
Output: The initial binding pose is the second pose in the 3D column and displayed without hydrogen.
[LiveDesign,MacroModel]
Schrodinger 20.4.3

Add to LiveReport

LiveDesign Admin

Home > Models

Select Model to change

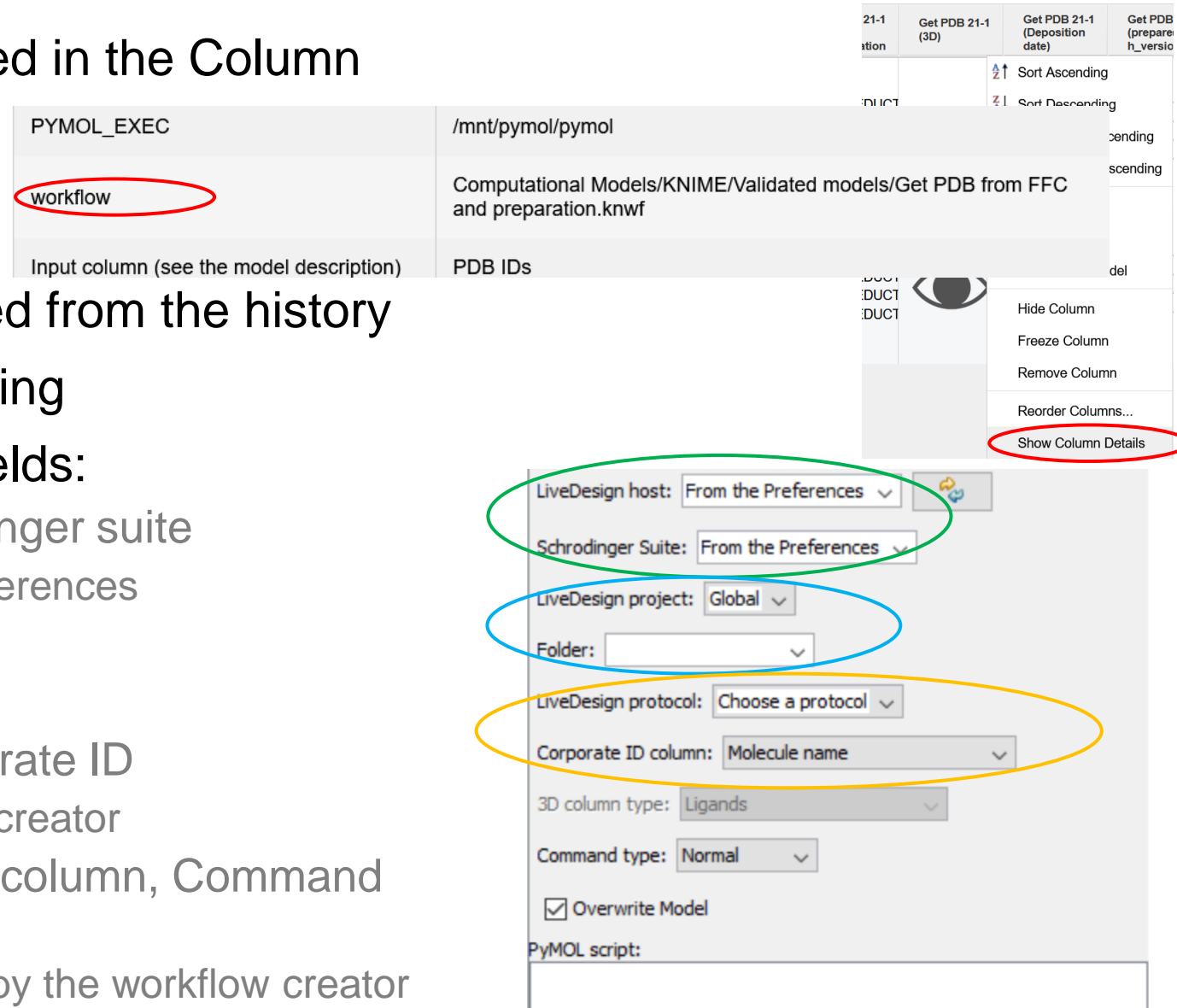
Q Get PDB from FFC Search 20 results (1106 total)

Action: ----- Go 0 of 20 selected

| <input type="checkbox"/> | NAME | DESCRIPTION | FOLDER |
|--------------------------|---------------------------------------|---|---|
| <input type="checkbox"/> | Get PDB from FFC | 2020/12/15 11:42:34 --- Get PDB from a FFCColumn : Downloads the structure for the PDB IDs listed in the selected Free Form Column from the LiveReport, extracts and creates new columns with the structures and corresponding structural information. [LiveDesign] Schrodinger | Computational Models/KNIME/UploadTest |
| <input type="checkbox"/> | Get PDB from FFC | 2020/12/15 11:44:00 --- Get PDB from a FFCColumn : Downloads the structure for the PDB IDs listed in the selected Free Form Column from the LiveReport, extracts and creates new columns with the structures and corresponding structural information. [LiveDesign] Schrodinger | Computational Models/KNIME/From the Hub |
| <input type="checkbox"/> | Get PDB from FFC and preparation 21-1 | 2021/01/06 11:01:12 --- Get PDB from a FFCColumn and Protein preparation : Input column: PDB IDs in a Free Form Column Downloads the structure for the PDB IDs listed in the selected Free Form Column from the LiveReport, optionally prepare the structures, extracts and creates new columns with the structures and corresponding structural information. [LiveDesign,PPrep] Schrodinger 21.1.0 | Computational Models/KNIME/Validated models |
| <input type="checkbox"/> | Get PDB from FFC and preparation | 2021/01/06 11:04:57 --- Get PDB from a FFCColumn and Protein preparation : Input column: PDB IDs in a Free Form Column Downloads the structure for the PDB IDs listed in | Computational Models/KNIME/Validated models |

Upload as LiveDesign model – other usability improvements

- The model folder and name are stored in the Column details
 - Especially convenient for the Parametrized models
- The Folder field value can be selected from the history
- The workflow is saved before uploading
- Reordered the configuration panel fields:
 - **Machine specific** - Host and Schrodinger suite
 - Mandatory, but ideally from the preferences
 - **Model location** - Project and Folder
 - can keep the defaults
 - **Workflow input** - Protocol and Corporate ID
 - mandatory, but set by the workflow creator
 - Workflow execution and output - 3D column, Command type, Overwrite and PyMOL
 - Optional, workflow specific and set by the workflow creator

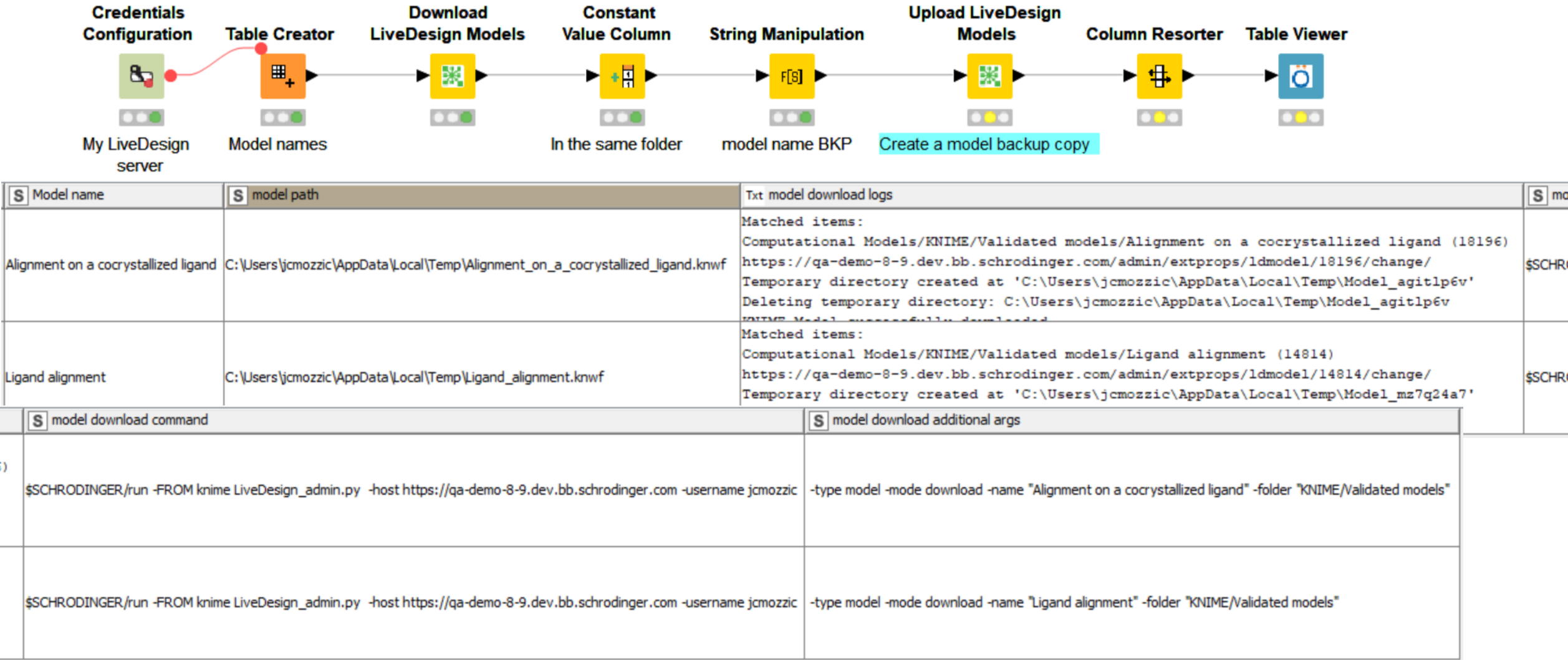


LiveDesign model and protocol administration nodes

- Nodes to upload, download and verify
 - Operate on a list of model or protocol names or files
- Application examples:
 - Create backup copies of some models before they are updated
 - Create a model or protocol copy for testing changes and only visible from a specific project
 - Copy from a testing to a production LiveDesign instance
 - Deploy the latest version of the validated models available from the KNIME hub
 - Deploy the latest version of the generic KNIME protocols
 - Compare 2 versions of a protocol or a model
- Run LiveDesign_admin.py script
 - The command lines are reported in the node output table.
So they can be run in a shell if the LiveDesign host isn't accessible from the KNIME session
 - **The script can also be used on non-KNIME models and protocols**

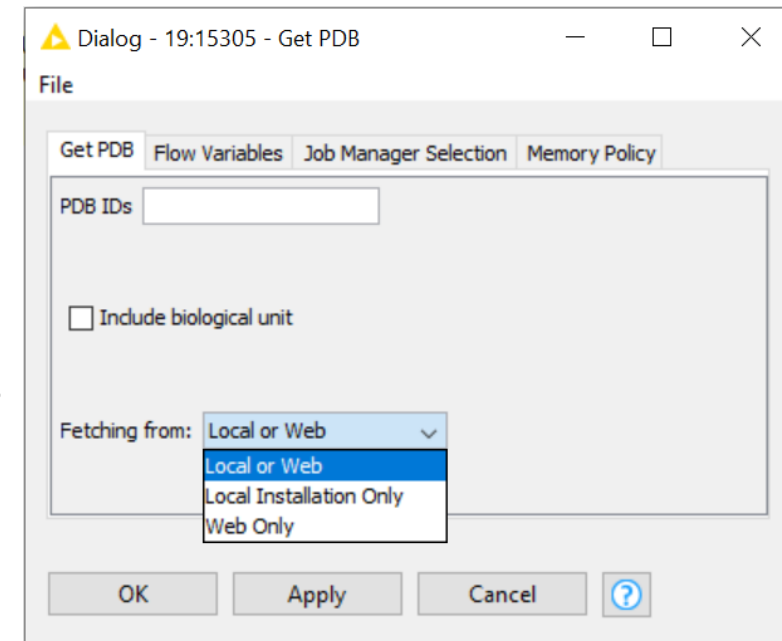
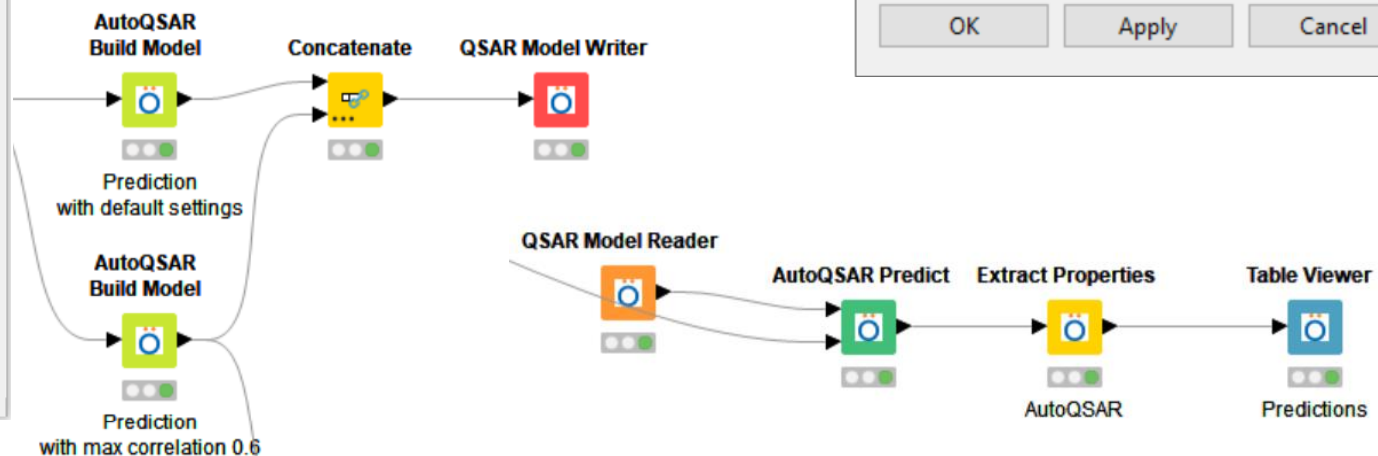
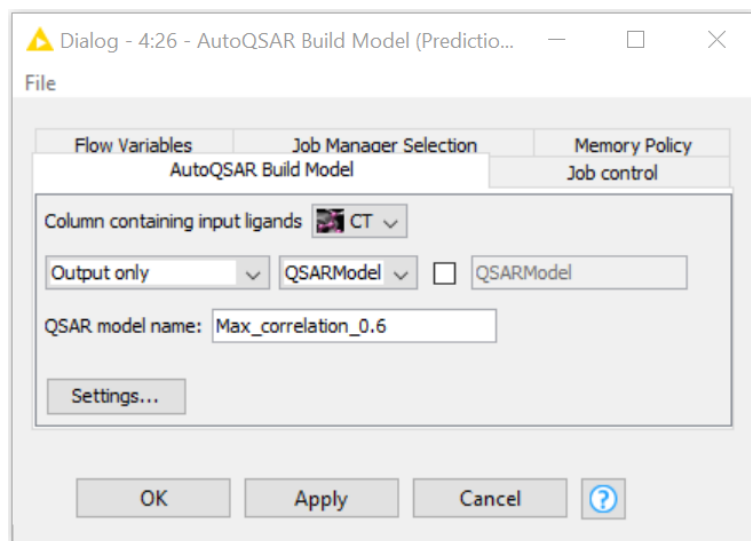
LiveDesign administration nodes – application example

- Create backup copies of some models



Minor improvements

- In the Get PDB node, include the biological unit and set the source from the configuration panel
- The Jaguar minimization node runs on multiple CPUs
- Customize the model names in the AutoQSAR Build Model node
 - Document the experiments and write them as separate files

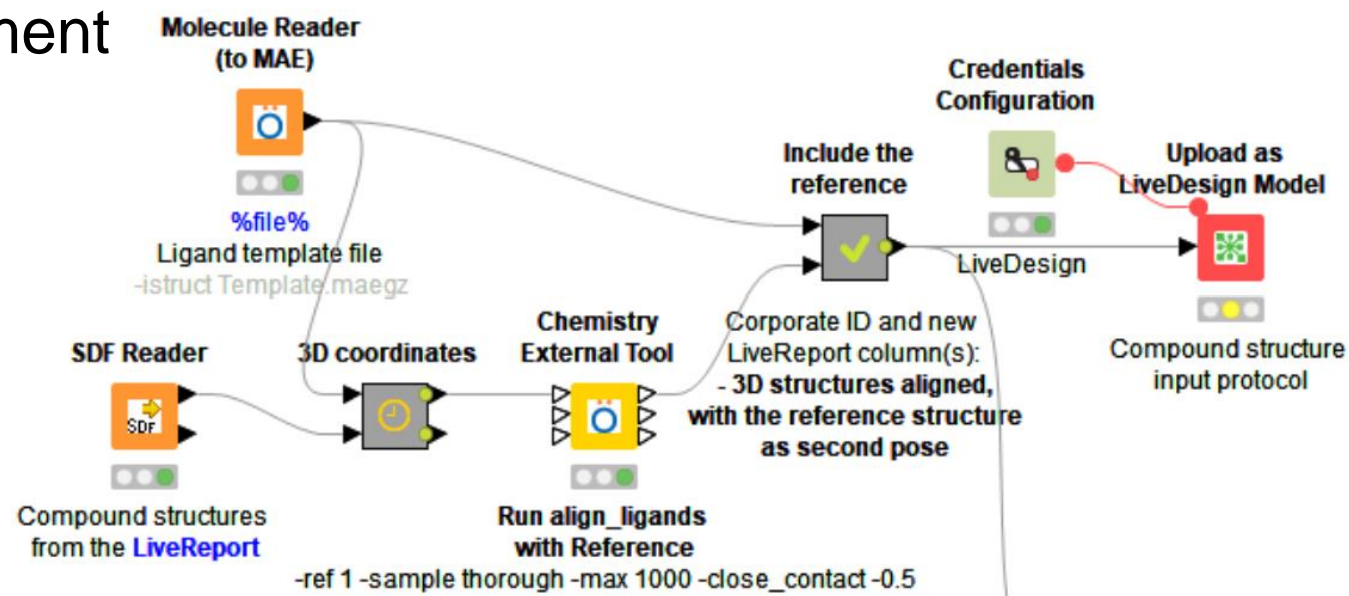


Components and Workflow Examples

- Cheminformatics – AutoQSAR: with model renaming
- LiveDesign administration
 - Create backup or testing model copies
 - Add the latest version of the validated models and generic KNIME protocols
 - Compare versions of a protocol or a model

LiveDesign models:

- Structure alignment – Ligand alignment
 - with a cocrystallized reference
 - Using align_ligand utility

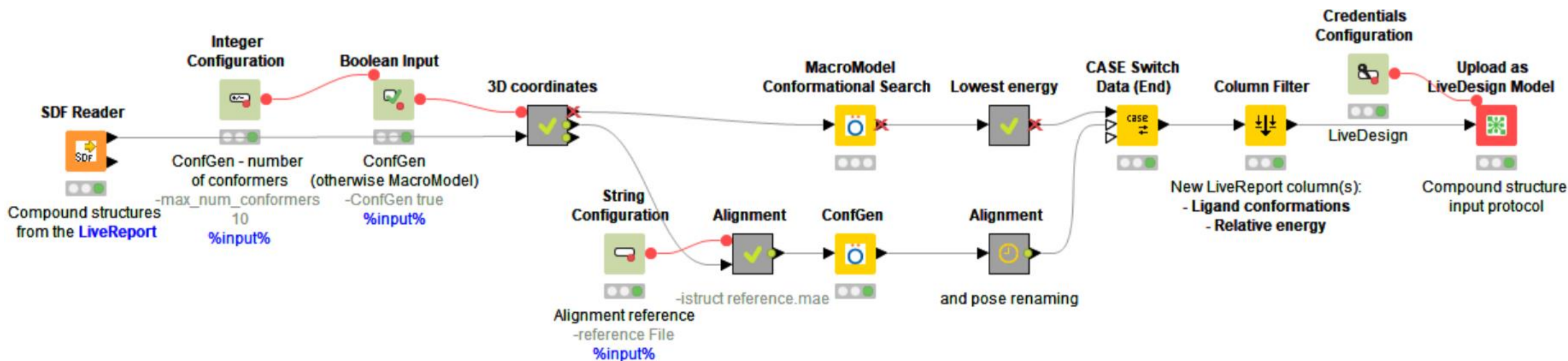


Components and Workflow Examples

Improved LiveDesign models:

- Low energy conformations

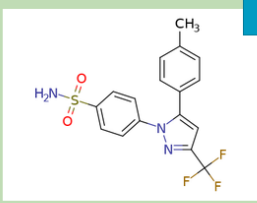

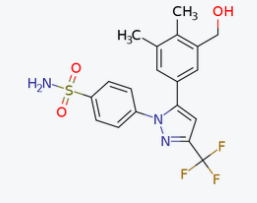

- Runs a MacroModel or ConfGen conformational search on the Compound structure column structures from the LiveReport, prepared with LigPrep.
- The lowest energy conformations are reported back in the LiveReport as poses as well as a column with the corresponding relative energies. These are also included in the pose name.
- The conformational search method and number of conformers can be controlled from LiveDesign admin panel or from the Parameterize model panel.



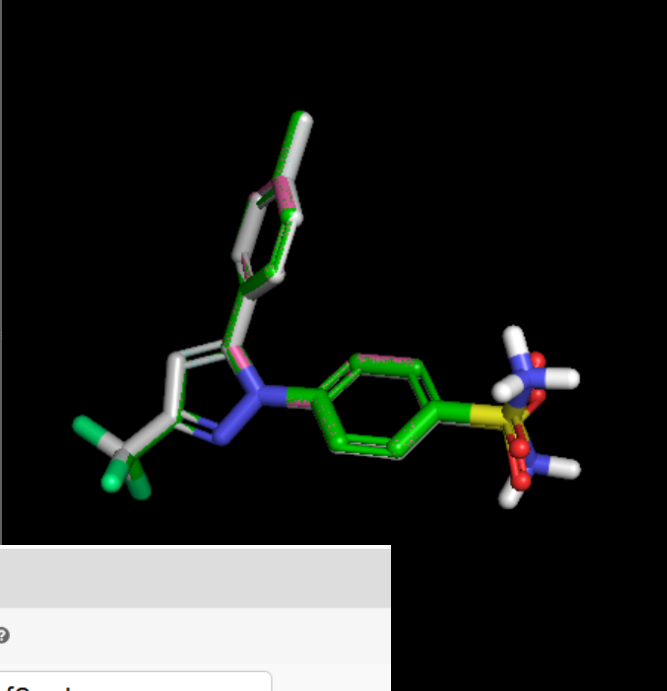
Low energy conformations

- The conformations and the ligands are aligned
- Pose name: conformer ID, relative energy

Open Live Report + 21-1 testing ▾

| <input type="checkbox"/> | Compound Structure | ID | Low energy conformation (3D) | Low energy conformation (Relative) |
|-------------------------------------|---|------------|---|---|
| <input checked="" type="checkbox"/> |  | CMPD-10409 |  | 0.0 0.006 0.007 0.007 0.126 0.282 0.313 0.571 More available... |
| <input type="checkbox"/> |  | V64860 |  | 0.0 0.14 0.449 0.483 0.769 0.995 1.031 1.082 More available... |

VISUALIZE + 3D ▾



Contents Styles

MODEL:

☒ Low energy conformation (3D)

☒ CMPD-10409 (10 poses) ▾

☒ 0_0.0_1743076806 ●

☒ 1_0.006_615768295 ●

☒ 2_0.007_1174613324 ●

☒ 3_0.007_1756598433 ●

☐ 4_0.126_855777056 ●

☐ 5_0.282_1894630593 ●

☐ 6_0.313_443848968 ●

☐ 7_0.571_1660388703 ●

☐ 8_1.153_1356054653 ●


☐ 9_1.169_1812412864 ●

☐ 1 (3D)

☐ 1 (3D)

☐ 1 (3D)

TOOLS: FIT:



MODEL DATA

| NAME | PARAMETER TYPE | DATA ⓘ |
|--------------------------|----------------|--|
| extra argument 3 | Text | -ConfGen true |
| extra argument 1 (60370) | | |
| extra argument 1 | Text | -istruct reference.mae |
| extra file 1 | File | Parent File: <i>mockup.txt</i> Currently: <i>reference.mae</i> <input type="checkbox"/> Clear Change: <input type="button" value="Browse..."/> No file selected. |

The workflow parameters and reference file can be controlled either from the model Admin page or from the Parametrize model panel.

Get PDB from a FFColumn and Protein preparation

COX DATA & COLUMNS Open Live Report PDB

Project LiveReport

Computational Models

- KNIME
- Validated models
- Get PDB from FFC and PPRep

3D

- Chain list
- Deposition date
- PDB classification
- PDB title
- prepared_with_version
- Resolution

Compound Structure

Get PDB from FFC and preparation

Modified January 20, 2021 by jcmozzic
2021/01/18 15:37:09
--- Get PDB from a FFColumn and Protein preparation :

Input column: PDB IDs in a Free Form Column

Downloads the structure for the PDB IDs listed in the selected Free Form Column from the LiveReport, optionally prepare the structures, extracts and creates new columns with the structures and corresponding structural information. The sstructure source, preparation and alignment steps can be controlled from LiveDesign admin panel.

[LiveDesign,PPRep]
Schrodinger 20.4.1

Add to LiveReport

Parameterize Model

Name: Test

Description: 2021/01/18 15:37:09
--- Get PDB from a FFColumn and Protein preparation :

Model Data

Input column: PDB IDs Change Column...

extra argument 1: -preparationORnot preparation

extra file 3: 1CX2 with V49629 docked with constraints.pdb Upload File...

☐ Publish(share data between Live Reports)(?)

Contents **Styles**

MODEL:

- ☒ A mini (3D)
- ☒ V38532 (1 pose)
- ☒ Row1_1977711137
- ☒ A not (3D)
- ☒ V38532 (1 pose)
- ☒ Row1_460132198
- ☐ 3 cocryst (3D)
- ☐ A prep (3D)
- ☐ Ensemble docking (3D)
- ☐ Get PDB (3D)
- ☐ Get PDB from FFC (3D)
- ☐ No PPRep (CT - DELETED)
- ☐ Not (CT - DELETED)
- ☐ PPRep (CT - DELETED)
- ☐ PPRep - not (CT - DELETED)
- ☐ Preparation (CT - DELETED)

LiveDesign Admin WELCOME, DEMO, STATUS / HELP / LOG OUT

Home > Models > Get PDB from FFC and PPRep (18271)

Change Model ARCHIVE HISTORY

ID: 18271

Name: Get PDB from FFC and PPRep

Give this a short and descriptive name that modelers will understand

MODEL DATA

| NAME | PARAMETER TYPE | DATA | PARAMETER SOURCE |
|--------------------------|----------------|----------------------------|------------------|
| extra argument 1 (48323) | | | |
| extra argument 1 | Text | -preparationORnot preparat | Set Fixed |
| Input column (48324) | | | |



New features in the KNIME extension

In Schrödinger Suite 2020-4

KNIME in LiveDesign

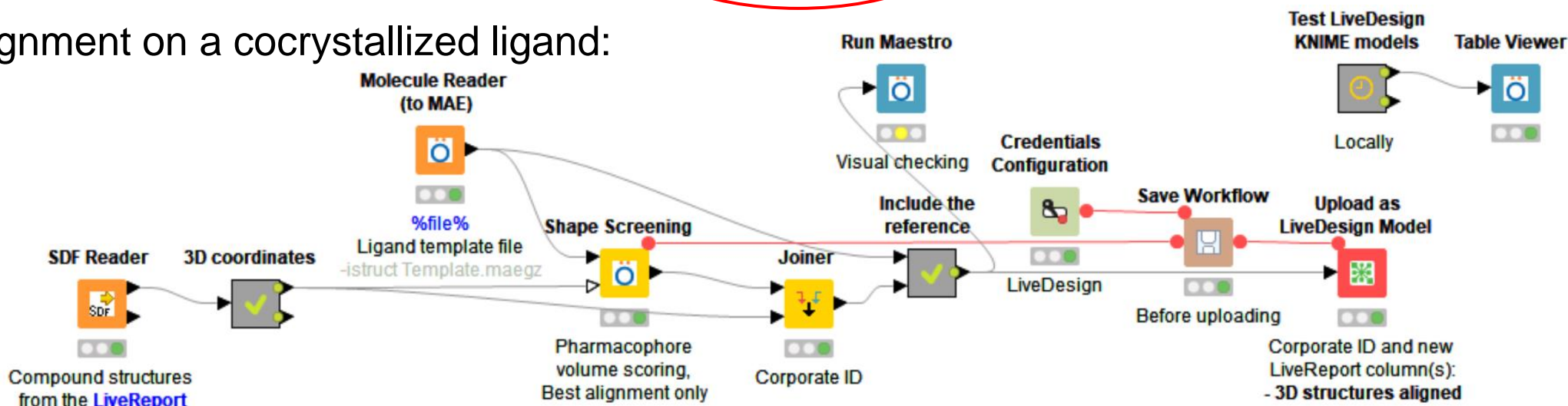
- System specific files and workflow parameters can be **changed on the LiveDesign admin page**
- **Preferences** for faster configuration of the Upload as LiveDesign model node
- Surfaces rendering can be controlled and the models deployed to a specific LiveDesign project
- Use nodes from extensions not included in the default installation
- The Prime Build Homology Model node accepts any Parameter flow variable
- New Job Monitor node

Generic protocols – Admin page new settings

- System specific files can be changed from LiveDesign admin page
 - No need to open KNIME, nor set it each time in the Parameterize model configuration panel
 - eg ligand alignment template, Glide grid, QSAR model file
 - The corresponding KNIME_batch.py arguments have to be added to the page too
 - See Batch test node output

| MODEL DATA | | | |
|------------------|----------------|---|--|
| NAME | PARAMETER TYPE | DATA ? | PARAMETER SOURCE |
| extra file 1 | File | Parent File: <i>mockup.txt</i> Currently: <i>Template.maegz</i> <input type="checkbox"/> Clear Change: <input type="button" value="Browse..."/> No file selected. | <input type="text" value="Set Fixed"/> |
| extra argument 1 | Text | <input type="text" value="-istruct Template.maegz"/> | <input type="text" value="Set Fixed"/> |

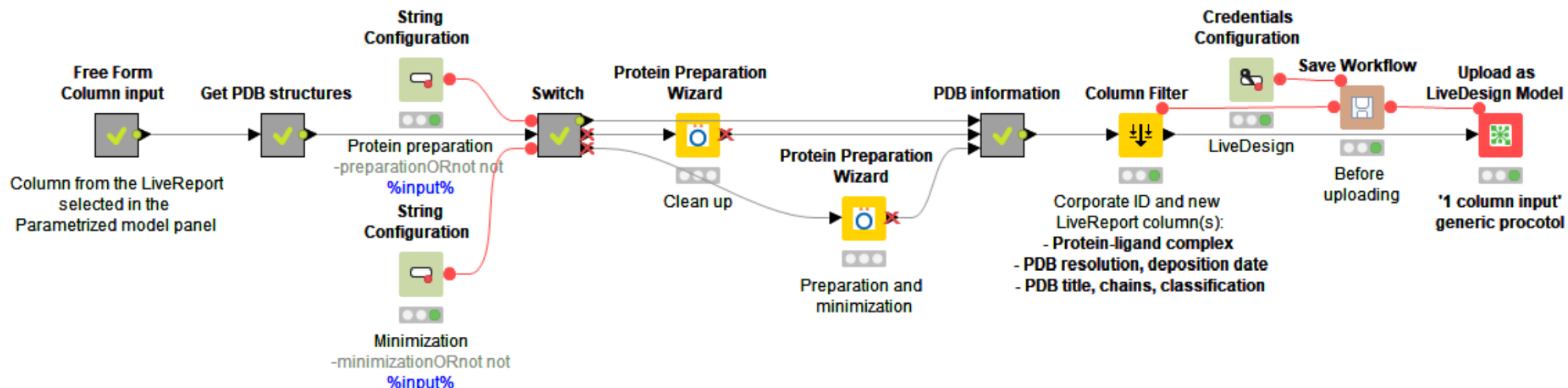
Alignment on a cocrystallized ligand:



Generic protocols – Admin page new settings

- Workflow parameters
 - Using the extra argument fields
eg Get PDB and preparation

| MODEL DATA | | |
|--------------------------|----------------|--|
| NAME | PARAMETER TYPE | DATA ⓘ |
| extra argument 1 (48323) | | |
| extra argument 1 | Text | <input type="text" value="-preparationORnot preparati"/> |



- Use a specific queue

Queue eg #te_queue=knime or echo "default queue"

Text

- The KNIME model calculations are distributed according to the Batch size

Generic protocols – Admin page new settings

COX

DATA & COLUMNS

Project LiveReport

PPrep

Computational Models

KNIME

Validated models

Get PDB from FFC and PPrep

3D

Chain list

Deposition date

PDB classification

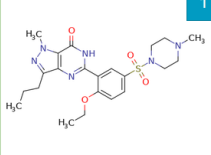

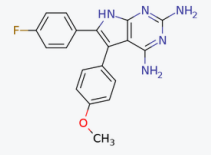

PDB title

prepared_with_version

Resolution

Open Live Report

PDB

| | Compound Structure | ID | A mini (Chain list) | A mini (Resolution) | A mini (PDB classification) | A mini (3D) | A mini (Deposition date) | A mini (prepared_with_version) | A mini (PDB title) |
|---|---|---------|---------------------|---------------------|-----------------------------|---|--------------------------|--------------------------------|---|
| 1 |  | V38532 | L, H | 2.2 | HYDROLASE/H INHIBIT |  | 06-JUL-92 | 2020-4 | REFINED 2 ANGSTROM X-RAY CRYSTAL STRUCTURE BOVINE THROMBIN COMPLEX FORMED WITH BENZAMIDINE More available... |
| 2 |  | V222790 | L, H | 2.5 | HYDROLASE/H INHIBIT |  | 06-JUL-92 | 2020-4 | REFINED 2 ANGSTROM X-RAY CRYSTAL STRUCTURE BOVINE THROMBIN COMPLEX FORMED WITH BENZAMIDINE More available... |

LiveDesign Admin

WELCOME, DEMO, STATUS / HELP / LOG OUT

Home > Models > Get PDB from FFC and PPrep (18271)

Change Model

ARCHIVE HISTORY

ID: 18271

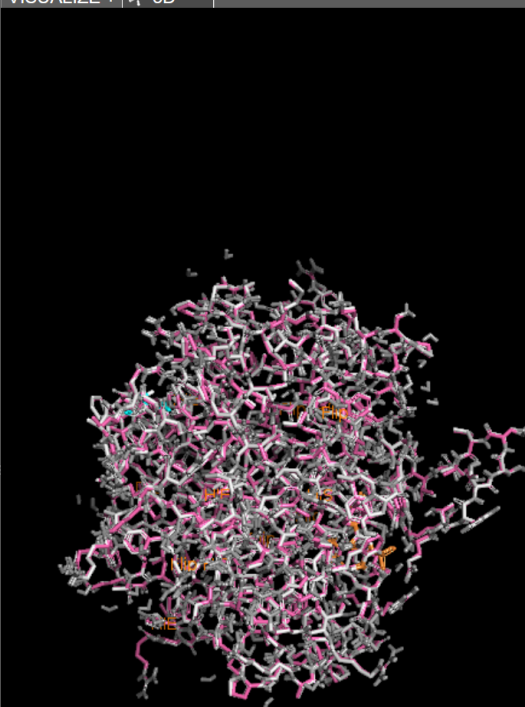
Name: Get PDB from FFC and PPrep

Give this a short and descriptive name that modelers will understand

| MODEL DATA | NAME | PARAMETER TYPE | DATA | PARAMETER SOURCE |
|--------------------------|------|----------------|----------------------------|------------------|
| extra argument 1 (48323) | | | | |
| extra argument 1 | | Text | -preparationORnot preparat | Set Fixed |
| Input column (48324) | | | | |

Give Feedback

Visualize + 3D



Contents

Styles

MODEL:

A mini (3D)

V38532 (1 pose)

Row1_1977711137

A not (3D)

V38532 (1 pose)

Row1_460132198

3 cocryst (3D)

A prep (3D)

Ensemble docking (3D)

Get PDB (3D)

Get PDB from FFC (3D)

No PPrep (CT - DELETED)

Not (CT - DELETED)

PPrep (CT - DELETED)

PPrep - not (CT - DELETED)

Preparation (CT - DELETED)

Thrombin Docking (3D)

Thrombin WaterMap (3D)

TOOLS:

FIT:

Extra KNIME extensions

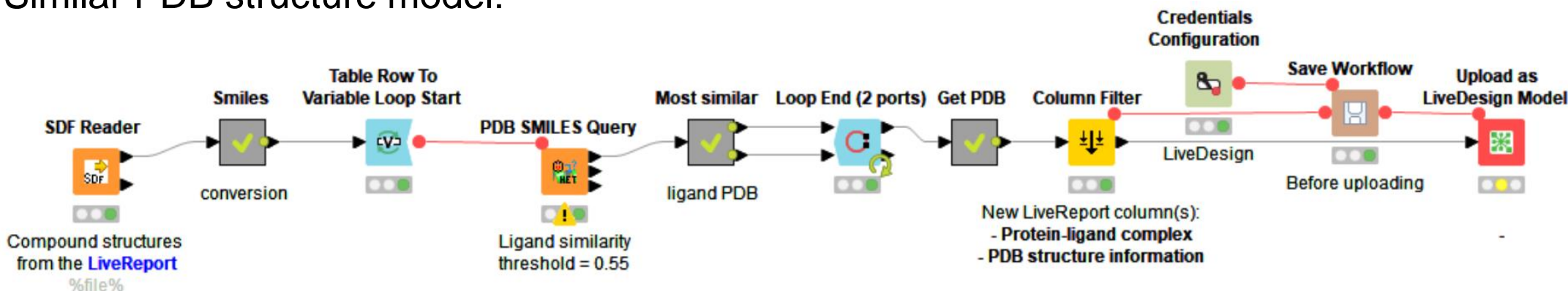
- For workflow using nodes from extensions not included in Schrodinger default installation
 - eg Vernalis, Erlwood (Lilly) nodes
- Run KNIME_install.py -configuration
 - Add the extensions on the fly
 - In the Protocol command
 - Store the extra extensions in a common location

COMMAND

ID 6968

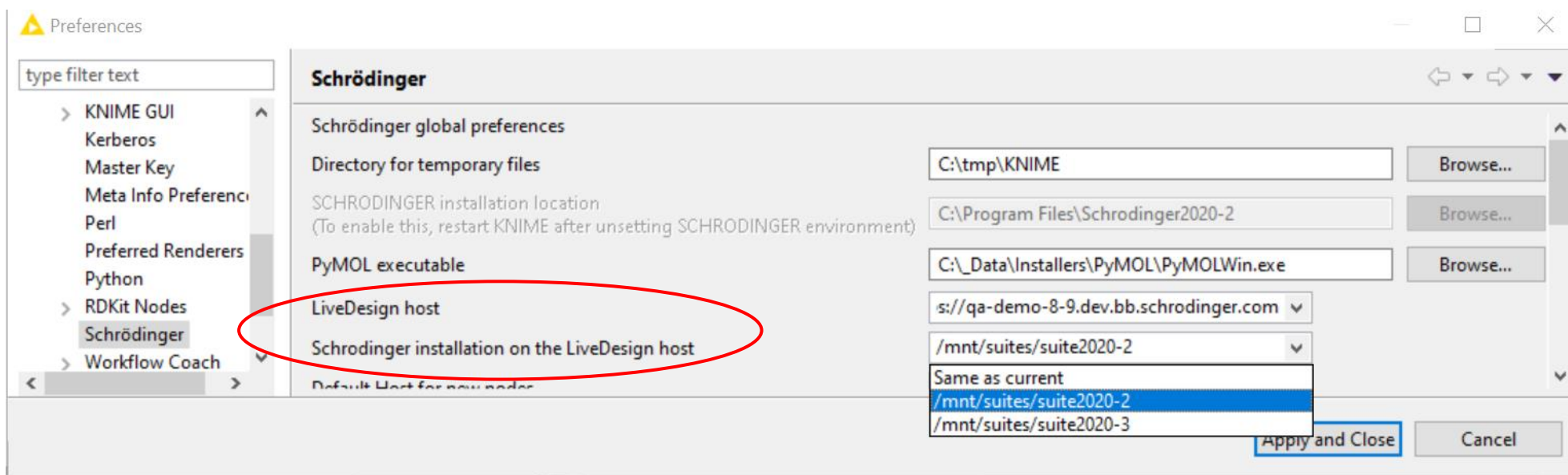
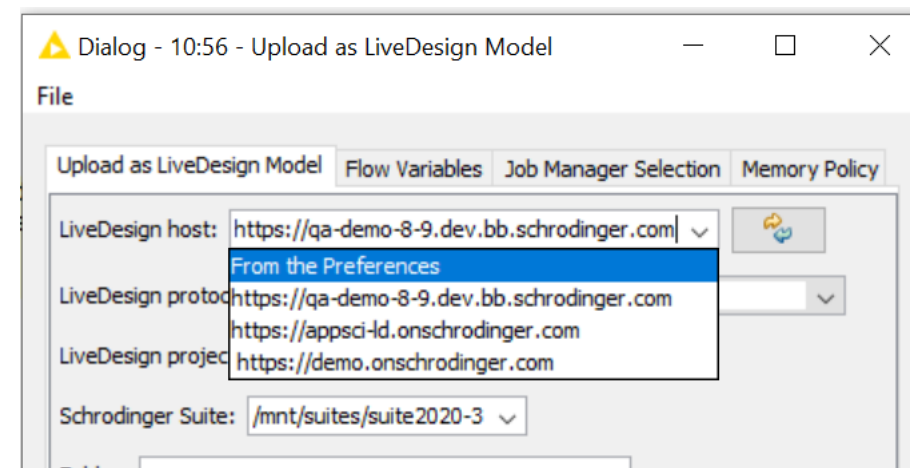
```
$SCHRODINGER/run -FROM knime KNIME_install.py -features_list  
${extra_extensions:FILE-INPUT} -verbose -keeplogs -configuration  
$PWD/ExtraExtensions/configuration "$SCHRODINGER/" -ls -1  
"$SCHRODINGER" | grep knime-v"/bin/Linux-x86_64/knime"  
$SCHRODINGER/run KNIME_batch.py $workflow:FILE-INPUT -run -isdf  
@/SDF-FILE-List-derr $/KNIME -line-verbosity:TEXT-INPUT  
argument 2: FILE-INPUT } $extra_argument 3: FILE-INPUT } -data  
workspace -configuration $PWD/ExtraExtensions/configuration  
touch $extra_file 4: FILE-INPUT }
```

eg Similar PDB structure model:



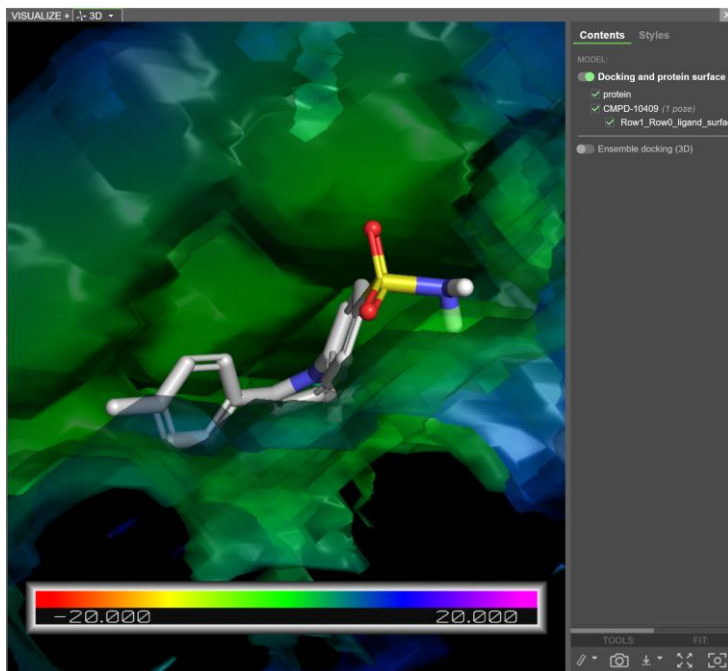
Upload as LiveDesign model node – Preferences

- Set the LiveDesign host and Schrodinger installation used the most often in the Preferences
 - And From Preferences in the node
 - Changed in one place when a new release is installed
 - Simplified configuration: only 2 workflow specific settings to configure for each workflow
- Switch easily between hosts or installations using history lists



Upload as LiveDesign model node – Surface rendering

- PyMOL script section to control the surface rendering
 - eg surface coloring
 - PyMOL Python commands



Manage Surfaces

| In | Limit | Entry | Volume Name | Vol | Surface Name | Comments | Surface Type | Isovalue | Area | Sigma |
|----|-------|---------|-------------|-----|--------------|----------|--------------|----------|----------|-------|
| | | 1: 1BL7 | surf | | surf_surf | surf | | 1 | 1920.711 | |

Import... Duplicate Delete Split Limit... Export to Map... Display Options... Volume Editor... Preferences...

Isovalue:

☐ Display at most: 16 Å²

Dialog - 4:456 - Upload as LiveDesign Model ('1 col...

File

Upload as LiveDesign Model | Flow Variables | Job Manager Selection | Memory Policy

LiveDesign host: From the Preferences

LiveDesign protocol: KNIME Workflow 20-4 - 1 column input (18092)

LiveDesign project: Global

Schrodinger Suite: From the Preferences

Folder: KNIME/Validated models

Corporate ID column: Corporate ID

3D column type: Ligands

Command type: Normal

☒ Overwrite Model

PyMOL script:

```
cmd.ramp_new("surf","CT",range=[-20,20],color=["red","yellow","green","blue","magenta"])
cmd.set("surface_color","surf","Surface*")
```

Table "default" - Rows: 4 | Spec - Columns: 4 | Properties | Flow Variables

| Row ID | CT | Molecule name | docking score | Surface |
|-----------|-----------------------------|---------------|---------------|----------------------------|
| Row0_Row0 | Molecule: 1BL7 #atoms: 5... | | | Surface: size=445000 by... |
| Row1_Row0 | Molecule: V64719 #atoms:... | V64719 | -5.547 | Surface: size=445000 by... |
| Row2_Row0 | Molecule: V64721 #atoms:... | V64721 | -4.684 | Surface: size=445000 by... |
| Row3_Row0 | Molecule: V64713 #atoms:... | V64713 | -4.555 | Surface: size=445000 by... |

OK Apply Cancel ?

Upload as LiveDesign model node – for a specific project

- The model can be exposed to a specific project only
 - eg Docking models for the target, local QSAR model
- Models with the same name can be uploaded to LiveDesign with the node provided they are added to different folders

Dialog - 7:15253 - Upload as LiveDesign Model (Ne... - □ ×

File

Upload as LiveDesign Model | Flow Variables | Job Manager Selection | Memory Policy

LiveDesign host: From the Preferences ▾

LiveDesign protocol: KNIME Workflow 20-4 (18091) ▾

LiveDesign project: HIV_Protease ▾

Schrodinger Suite: Same as current ▾

Folder: KNIME/Validated models

Corporate ID column: Molecule name ▾

3D column type: Ligands ▾

Command type: Normal ▾

☒ Overwrite Model

PyMOL script:

OK Apply Cancel ?

Minor Improvements and Fixes

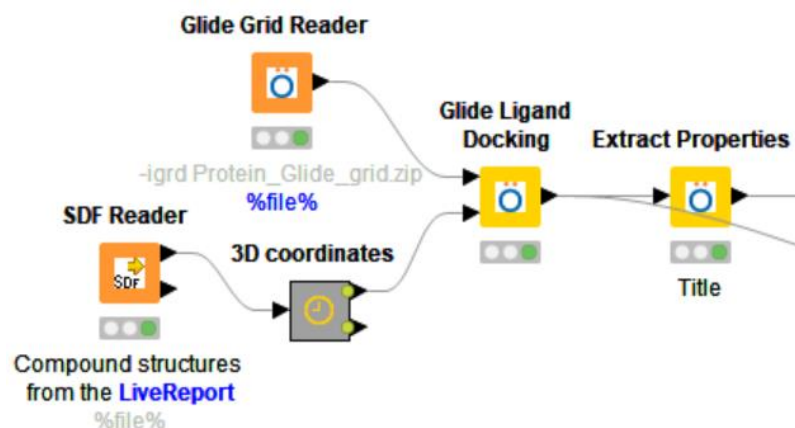
- The Prime Build Homology Model node accepts any command line options as Parameter flow variable
 - eg Variable name: PrimeBuild-MAX_INSERTION_SIZE, PrimeBuild-TAILS
- New Job Monitor node
 - Opens the same Job monitor panel as Maestro

Components and Workflow Examples

- KNIME LiveDesign models

- Alignment on a cocrystallized ligand
- Get PDB and protein preparation
- Binding pose strain, Docking and ligand strain
- Related PDB structures
- Docking and protein surface – with the surface coloring
- Models adapted to take system specific files from the Admin panel: Random forest, Ligand alignment, Pharmacophore screening and Docking models.

Available from: https://hub.knime.com/schroedinger/spaces/LiveDesign_models/latest



| MODEL DATA | | | |
|--------------------------|----------------|---|--|
| NAME | PARAMETER TYPE | DATA | PARAMETER SOURCE |
| extra argument 1 (50397) | | | |
| extra argument 1 | Text | <input type="text" value="-igrd Protein_Glide_grid.zip"/> | <input type="text" value="Set Fixed"/> |
| extra file 1 (50399) | File | Parent File: <i>mockup.txt</i> Currently: <i>Protein_Glide_grid.zip</i> <input type="checkbox"/> Clear Change: <input type="button" value="Browse..."/> No file selected. | <input type="text" value="Set Fixed"/> |



New features in the KNIME extension

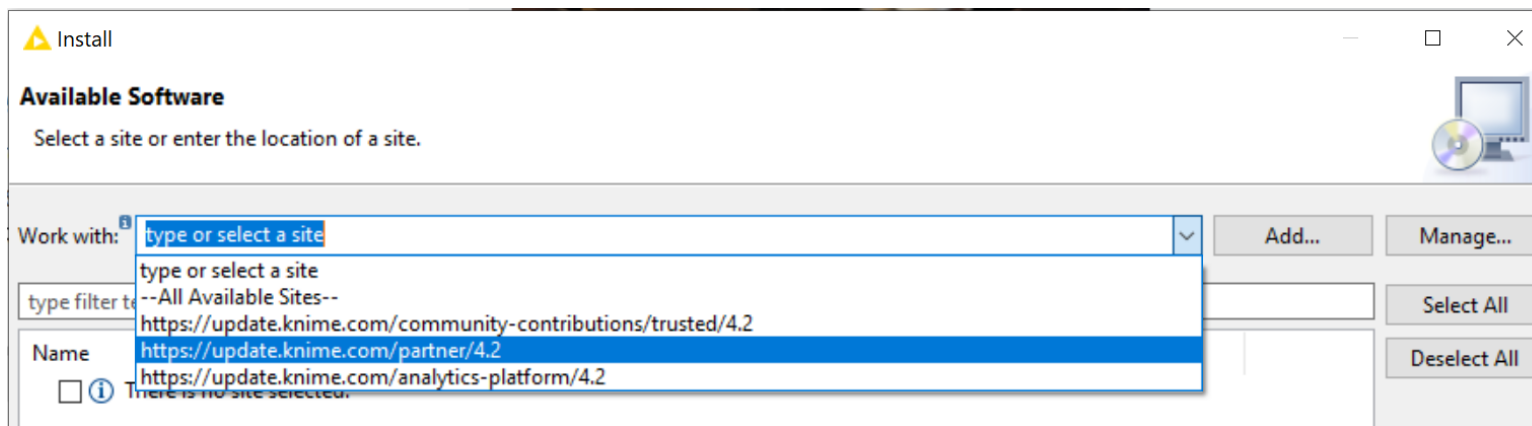
In Schrödinger Suite 2020-3

2020-3 New Features

- Supports the latest version of KNIME (v4.2, but includes v4.1.3)
- **Upload workflows as LiveDesign models**
 - **Generic protocol** taking any LiveReport column as input
 - **Pharmacophore hypotheses** can be added to the LiveReport
 - The models can be created in a specified folder under Computational model
 - The protocols and models can be **uploaded via a python script**
 - Option to avoid KNIME version incompatibilities
- **Any command line option** can be used in the **Glide ligand docking node**

KNIME 4.2

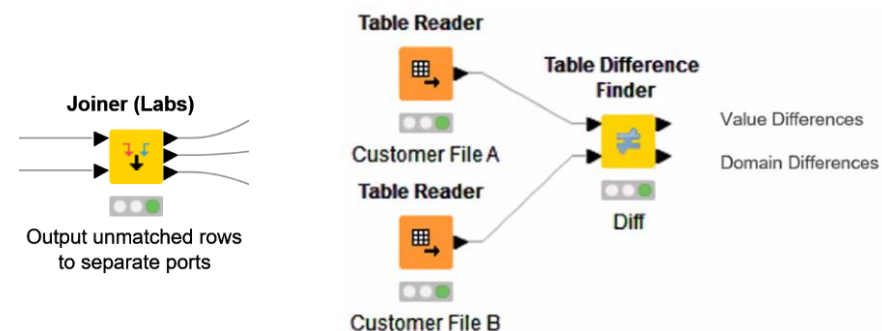
- KNIME 4.2 is supported with the Schrodinger extensions
 - But it doesn't run on old OS including CentOS 6
- KNIME 4.1.3 is embedded in Schrodinger installation
 - It can't be upgraded to KNIME 4.2 because of an Eclipse upgrade
- To run KNIME 4.2 from the Schrodinger Suite:
 - Make a stand alone installation: <https://www.knime.com/downloads/download-knime>
 - Add the Schrodinger nodes from the Partner update site or the zipped update site from the installation
 - Add -knimeInstallDir <path to KNIME 4.2 installation> to the icon command



KNIME Analytics Platform 4.2 – some new features

- KNIME Hub Community & Spaces
 - Spaces and User Profile Pages
- New Connector Nodes
 - Salesforce, SharePoint, Amazon DynamoDB, SAP Theobald
- Deep Learning – TensorFlow 2 Integration
- Performance Improvements
 - Python Speed-up, Simple File Reader, Joiner Node (unmatched output ports)
- New and improved Nodes
 - Table Difference Finder
 - String Manipulation (Multiple Column)
 - Dynamic Ports (Column Appender and Merge Variables nodes)

- CSV writer (Labs): no longer need to write KNIME URLs
- Database nodes



For Enterprise Data Science Challenges

- Integrated Deployment
- Elastic and Hybrid Execution
- Workflow Summary
- Guided Analytics - New WebPortal

See details in <https://www.knime.com/whats-new-in-knime-42>

Upload workflows as LiveDesign models – Generic protocols

- 2 Generic protocols
 - KNIME Workflow 20-3
 - Takes the 'Compound Structure' LiveReport column (ligands in 2D) as input
 - KNIME Workflow 20-3 - 1 column input
 - Takes 1 column from the LiveReport as input
eg a string, number, 3D structure or FEP map column
 - The column is selected in the Parametrized model panel when executing the model
 - Available as json files under: \$SCHRODINGER/knime-v5.1/data/
 - Use these as template to create customized protocols for specific scenarios
- -force_newer option
 - To add to the command to run workflows created with a newer version of KNIME
 - But ideally use the same (or more recent) KNIME version as used to create the workflow

Extra options eg -force_newer (36337)

Extra options eg -force_newer

Text

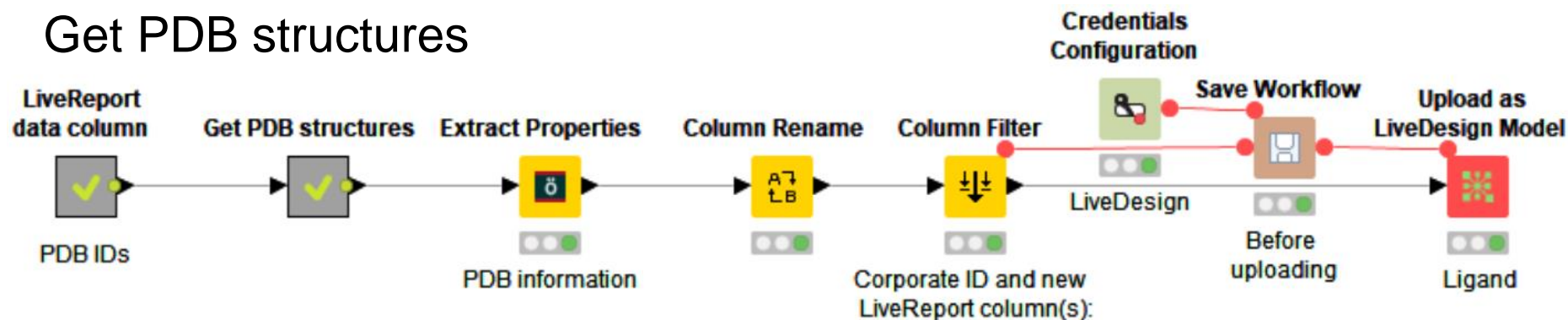
-debug -force_newer

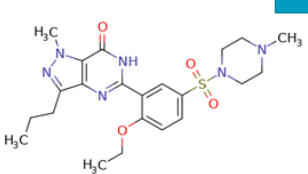

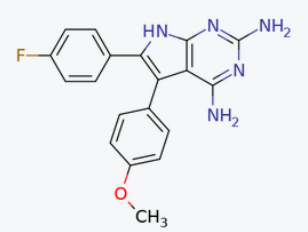

Set Fixed



Upload as LiveDesign model – Parameterized model examples

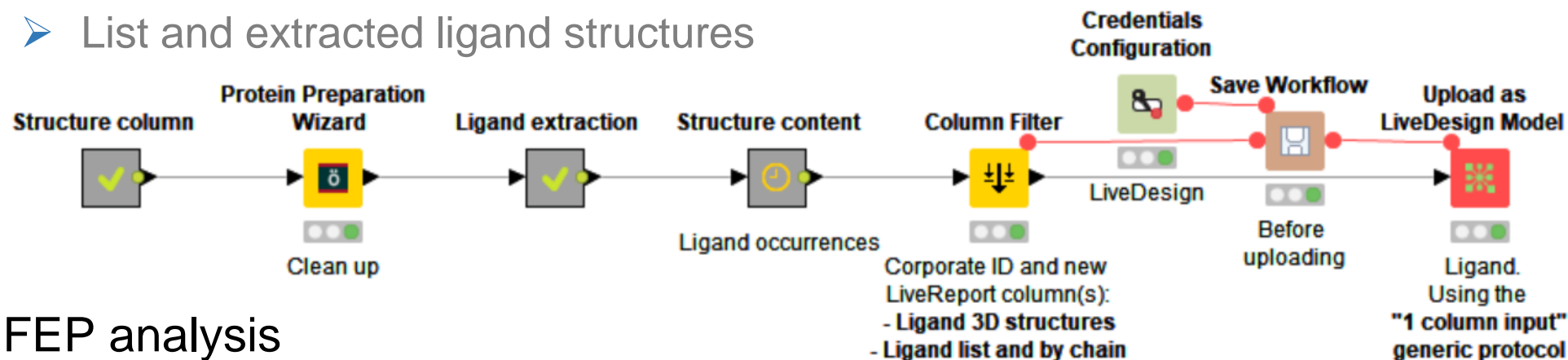
- Get PDB structures



| Open Live Report + PDB | | | | | | | | | | |
|------------------------|---|---------|-----------------|------|------------------------------|---|---------------------------|--|----------------------|----------------------|
| | Compound Structure | 1 ID | PDB ID (PDB ID) | FFC | Get PDB (PDB classification) | Get PDB (3D) | Get PDB (Deposition date) | Get PDB (PDB title) | Get PDB (Chain list) | Get PDB (Resolution) |
| 1 |  | V38532 | 1TBF 1TBF | 1ETR | HYDROLASE |  | 20-MAY-04 | CATALYTIC DOMAIN OF HUMAN PHOSPHODIESTERASE 5A IN COMPLEX WITH SILDENAFIL | A | 1.3 |
| 2 |  | V222790 | 4CMG | 4CMG | OXIDOREDUCT |  | 16-JAN-14 | CRYSTAL STRUCTURE OF PTERIDINE REDUCTASE 1 (PTR1) FROM TRYPANOSOMA BRUCEI IN TERNARY COMPLEX WITH COFACTOR AND INHIBITOR | A, B, C, D | 2.0 |

Upload as LiveDesign model – Parameterized model examples

- Cocrystallized ligands
 - From a PDB structure column
 - Protein preparation
 - List and extracted ligand structures



- FEP analysis
 - FEP map reader node
 - FEP map convergence information

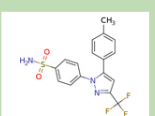

The screenshot shows the 'COX FEP' report interface. It includes a sidebar with navigation icons, a top bar with 'COX FEP' and 'Give Feedback', and a table of results. The table has columns for 'Compound Structure', 'ID', 'fmp FEP map (.fmp)', 'FEP1 (Energy Conv.)', 'FEP1 (CCC Conv.)', 'FEP1 (Lig. RMSD)', and 'FEP1 (REST Exch.)'. Two rows are visible, corresponding to compounds V217803 and V217804.

| | Compound Structure | ID | fmp FEP map (.fmp) | FEP1 (Energy Conv.) | FEP1 (CCC Conv.) | FEP1 (Lig. RMSD) | FEP1 (REST Exch.) |
|---|--------------------|---------|--------------------|---------------------|------------------|------------------|-------------------|
| 6 | | V217803 | | Fair | Good | Good | Fair |
| 7 | | V217804 | | Fair | Good | Good | Fair |

Upload as LiveDesign model node – Pharmacophore hypotheses

- A pharmacophore hypothesis column can be included in the output
 - Added to the 3D view along with the ligand hit

The screenshot displays the Schrödinger LiveDesign interface. On the left, a table lists compounds with columns for Compound Structure, ID, and various pharmacophore screening metrics. The first row is highlighted in green, showing compound CMPD-10409. To the right, a 3D visualization shows the ligand hit (CMPD-10409) in a 3D view, with a pharmacophore hypothesis overlaid. The hypothesis is represented by colored spheres (red for hydrogen bond donors, blue for hydrogen bond acceptors, and orange for hydrophobic regions) and arrows indicating the direction of the interactions. The interface also includes a 'Contents' panel on the right, showing the model details and a 'Tools' panel at the bottom.

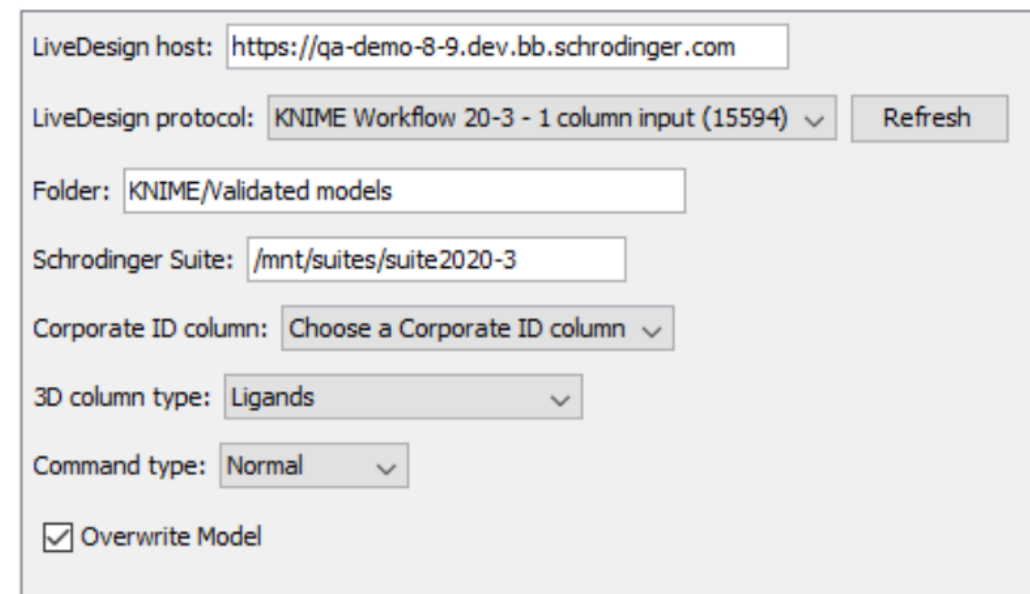
| Compound Structure | ID | Pharmacophore screening (HypoID) | Pharmacophore screening (Matched_Lig and_Sites) | Pharmacophore screening (Num_Sites_Matched) | Pharmacophore screening (PhaseScreen Score) | Pharmacophore screening (3D) |
|---|------------|----------------------------------|---|---|---|---|
|  | CMPD-10409 | AADPR_75 | A(3) A(2) D(4) P(-) R(10) | 4.0 | 1.626087411266 |  |

- Use 'LiveReport' as tag for the input SDF reader node
 - Taking Compound structures from the LiveReport as input
 - Case insensitive tag



Upload as LiveDesign model node – Folder

- The model location in the Computational model section in LiveDesign can be controlled when uploading the workflow
 - So as to keep the KNIME models organized
- Some improvements to make the Upload node and the model execution in LiveDesign more robust



The screenshot shows a configuration window for uploading a model to LiveDesign. It includes the following fields and controls:

- LiveDesign host:** A text input field containing the URL `https://qa-demo-8-9.dev.bb.schrodinger.com`.
- LiveDesign protocol:** A dropdown menu showing `KNIME Workflow 20-3 - 1 column input (15594)`, with a **Refresh** button to its right.
- Folder:** A text input field containing `KNIME/Validated models`.
- Schrodinger Suite:** A text input field containing `/mnt/suites/suite2020-3`.
- Corporate ID column:** A dropdown menu showing `Choose a Corporate ID column`.
- 3D column type:** A dropdown menu showing `Ligands`.
- Command type:** A dropdown menu showing `Normal`.
- Overwrite Model:** A checkbox that is currently checked.

Administration of KNIME models and protocols

- From LiveDesign Admin page
- Using LiveDesign_admin.py script
 - To upload Models and Protocols to a LiveDesign instance
 - No need to open the KNIME GUI. Easy for system administrators
 - Model deployment with 1 zip file and 1 command:

`“$SCHRODINGER”\run -FROM knime LiveDesign_admin.py`

`-type model -mode upload -username jcmozzic`

`-host https://demo.on.schrodinger.com -schrodinger /mnt/suites/suite2020-4`

`-file "Ligand_property_radar_plot.knwf"`

Also used to download, duplicate or verify Protocols and Models

- eg make a backup copy before updating, create a testing copy
 - Install the new version of the Validated models and generic KNIME protocols
- See options from `$SCHRODINGER/run -FROM knime LiveDesign_admin.py -h`

LiveDesign_admin.py script – application example

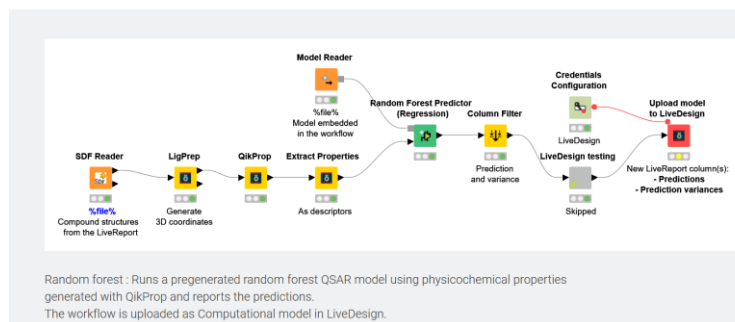
- https://hub.knime.com/schrodinger/spaces/Public/latest/LiveDesign_models
 - Ligand property radar plot
- “\$SCHRODINGER”\run -FROM knime LiveDesign_admin.py -host https://qa-demo-8-9.dev.bb.schrodinger.com -type protocol -mode **verify** -id 14322 -file “C:\tmp\KNIME\KNIME_Workflow_20-3.json” -username jcmozzic
- “\$SCHRODINGER”\run -FROM knime LiveDesign_admin.py -type **protocol** -mode upload -host https://qa-demo-8-9.dev.bb.schrodinger.com -name "KNIME Workflow 20-3" -schrodinger /mnt/suites/suite2020-3 -pymol_exec /mnt/suites/pymol_2_2-0/pymol -file “C:\tmp\KNIME\KNIME_Workflow_20-3.json” -username jcmozzic
 - C:\Program Files\Schrodinger2020-3\knime-v5.1\data\KNIME_Workflow_20-3.json
- “\$SCHRODINGER”\run -FROM knime LiveDesign_admin.py -host https://qa-demo-8-9.dev.bb.schrodinger.com -type model -mode **upload** -schrodinger /mnt/suites/suite2020-2 -file "C:\tmp\KNIME\Ligand_property_radar_plot.knwf" -name "Ligand property radar plot DEMO" -username jcmozzic

KNIME LiveDesign model files

- Standard KNIME workflow file
 - Zip file with .knwf extension
- LiveDesign subfolder
 - LiveDesign model and protocol information files
- Input file subfolder
 - A LiveReport sample input file
 - Other default input files that can be replaced to adapt the workflow to another system

Validated KNIME models ready to be installed on:
https://hub.knime.com/schroedinger/spaces/LiveDesign_models/latest/

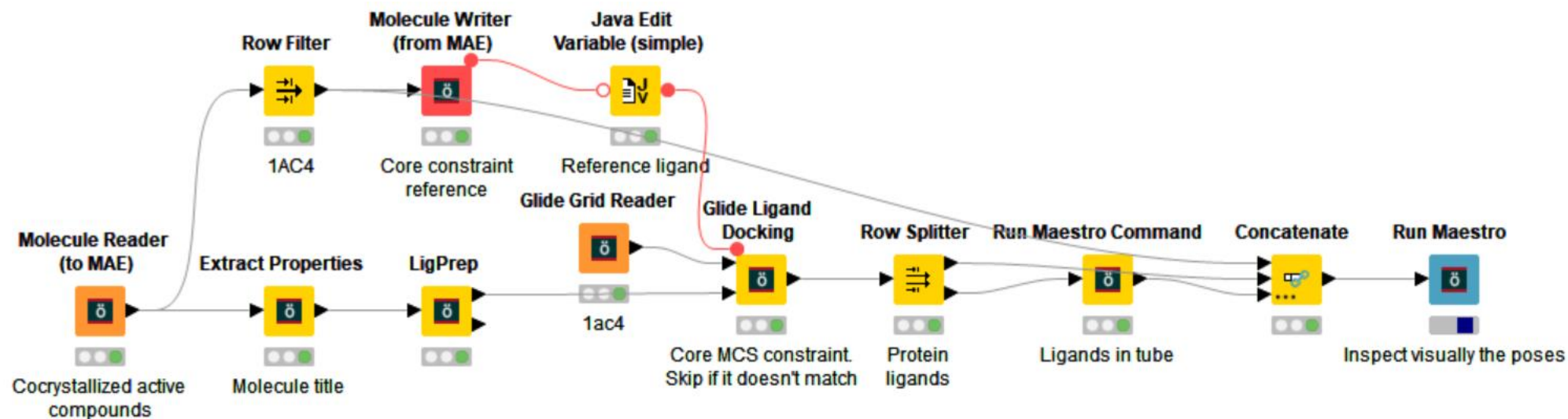
Random forest - to be run in LiveDesign



| | | |
|--|---------------------------------------|--|
| | ADME | |
| | Atropisomerism | |
| | Bioisosteres | |
| | Docking | |
| | Docking and protein surface | |
| | ESP surface | |
| | Ensemble docking | |
| | Installation test | |
| | Ligand CNS desirability plot | |
| | Ligand CNS desirability range plot | |
| | Ligand alignment | |
| | Ligand property radar plot | |
| | Low energy conformation | |
| | My workflow running on a KNIME server | |
| | Protonation forms | |
| | Random forest | |

Glide ligand docking – Parameter flow variables

- Any command line option can be used in the Glide ligand docking node



- Core reference ligand
- Loop over and test various docking parameters

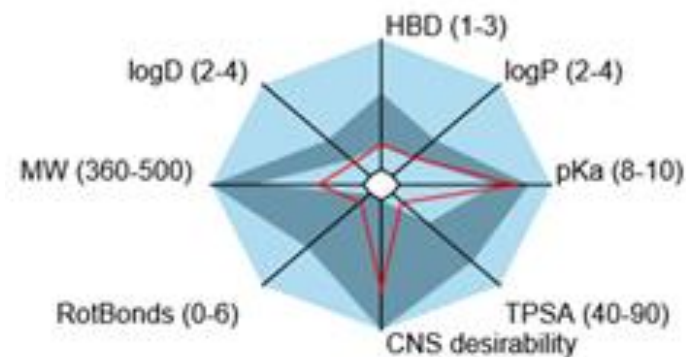
Components and Workflow Examples

- Available on https://hub.knime.com/schroedinger/spaces/Workflow_examples/latest/
- Docking – Core constraint and Loop over parameters – use the Parameter flow variables
- KNIME LiveDesign models

- CNS desirability radar range plot

Generates radar plots of the CNS desirability MPO properties and the number of rotatable bonds with the optimal property range.

- CNS desirability radar plot
- Pharmacophore search
- Atropisomerism
- Get PDB
- Cocrystallized ligands
- FEP analysis
- Available from: https://hub.knime.com/schroedinger/spaces/LiveDesign_models/latest





New features in the KNIME extension

In Schrödinger Suite 2020-2

2020-2 New Features

- The **3D structure type** (hence the rendering) and **execution mode** (automatic/click to run) can be controlled in the **Upload model to LiveDesign** node

Surfaces and images can be added to the LiveReport

- The Export image to LiveDesign node supports SVG images
- New **Prime Macrocycle Conformation sampling** node
- The Molecule reader node takes in cif format
- Some Components/Metanodes are available on the KNIME hub

Upload Model to LiveDesign – Configuration Panel

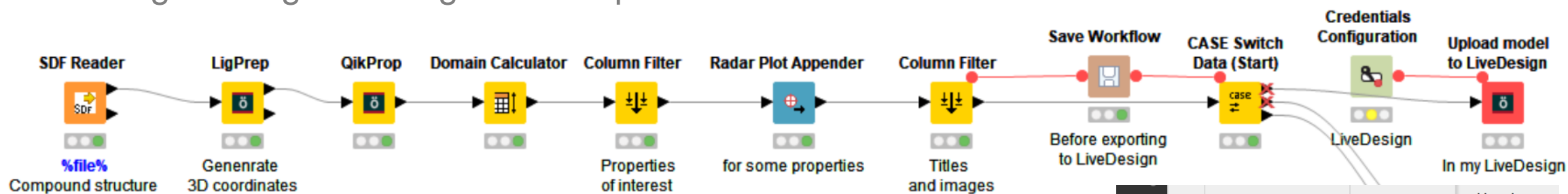
New fields to control:

- The 3D structure output type
 - So the LiveDesign uses a suitable rendering for ligands or pose viewer/protein structures
- The command type
 - Normal - The model is run automatically when added to the LiveReport
 - Click To Run - Each cell must be requested to run individually

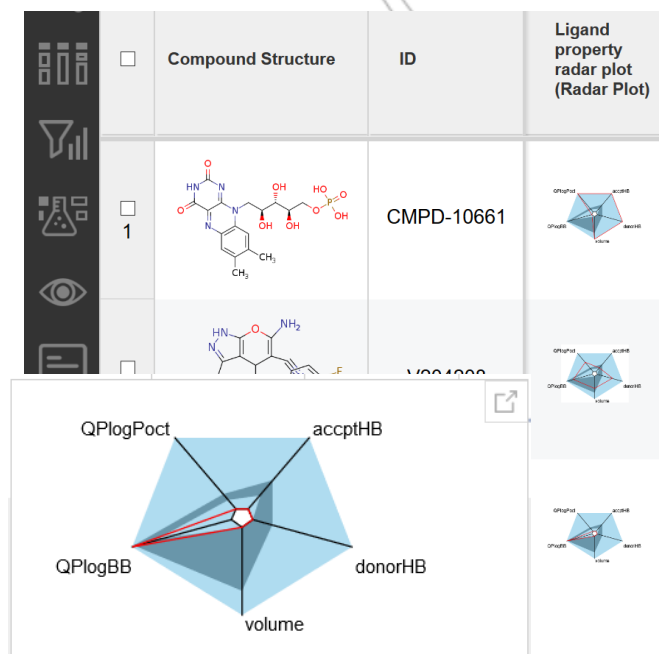
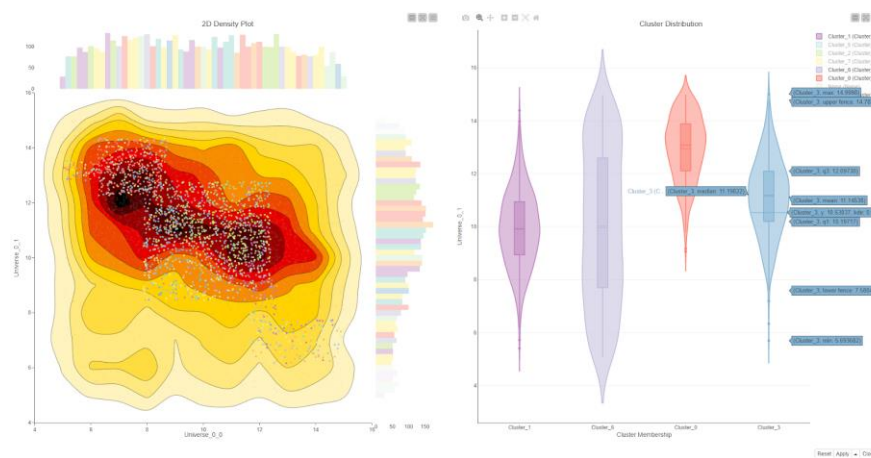
The screenshot shows a configuration dialog box titled "Dialog - 5:15247 - Upload model to LiveDesign (I...". The dialog has a "File" tab selected. Inside, there are two tabs: "Job Manager Selection" (active) and "Memory Policy". Under "Job Manager Selection", there is a sub-tab "Upload model to LiveDesign". The configuration fields include: "LiveDesign host" (text box with "https://qa-demo-8-9.dev.bb.schrodinger.com"), "LiveDesign protocol" (dropdown menu showing "KNIME Workflow 20-2 (14322)" with a "Refresh" button), "Schrodinger Suite" (text box with "/mnt/suites/suite2020-2-nb053"), "Corporate ID column" (dropdown menu showing "Molecule name"), "3D column type" (dropdown menu showing "Docked poses"), and "Command type" (dropdown menu showing "Normal"). At the bottom, there is a checked checkbox for "Overwrite model". The dialog has "OK", "Apply", "Cancel", and a help icon (?) buttons at the bottom.

Upload Model to LiveDesign – Images and Surfaces

- The ligand or protein structures can include a surface
- Image columns can be added to the LiveReport
 - eg The Ligand designer radar plots stored as a new column



- Export image to LiveDesign node supports SVG images
 - eg from the various KNIME plotting nodes and Plotly integration:



KNIME workflow run in LiveDesign – Pose viewer column

DATA & COLUMNS

Project LiveReport

Search columns

▼ Glide Docking Protocol_QA

▼ Glide Docking with LID

▼ GUI_DeepQSAR

▼ HSP90_WM

▼ Jaguar

▼ Kmeans Clustering and Ran...

▼ KNIME

Aniline Genotoxicity (Energ...

▼ Docking

▼ Docking and protein surf...

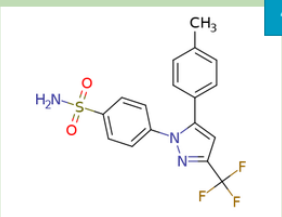

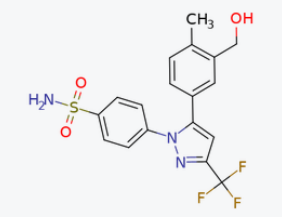
▼ Docking TMP

▼ Docking_

▼ DockingWithSurfaces

▼ DockingWithSurfaces-Mac

Open Live Report + Reception Review copy

| | Compound Structure | ID | Docking_ (3D) | Docking_ (docking score) |
|---|---|------------|---|--------------------------|
| 1 |  | CMPD-10409 |  | -5.3 |
| 2 |  | V5816 | | |

Job Manager Selection

Upload model to LiveDesign

Memory Policy

Flow Variables

LiveDesign host: <https://qa-demo-8-9.dev.bb.schrodinger.com>

LiveDesign protocol: KNIME Workflow 20-2 (14322) Refresh

Schrodinger Suite: /mnt/suites/suite2020-2-nb053

Corporate ID column: Molecule name

3D column type: Docked poses

Command type: Normal

☒ Overwrite model

OK Apply Cancel ?

Visualize + 3D

Contents

Styles

☐ COX1 (3D)

☐ COX2 (3D)

☐ Docking (3D)

☐ Docking and protein surf...

☒ Docking_ (3D)

☒ protein

☒ CMPD-10409

+ 1 pose

☐ Ensemble docking (3D)

☐ LD docking (3D)

☐ Protonation forms (3D)

+ Add 3D models to visualize selected compounds. Click here, then browse or search for any models containing the word '(3D)' in the list that appears on the left.

Export

Glide Grid Reader

Glide Ligand Docking

Extract Properties

Ensemble docking

Title

SDF Reader

LigPrep

Generate 3D coordinates

Compound structure column (2D) from the LiveReport

Column Filter

Only relevant columns for the Live Report

Configuration

LiveDesign

Upload model to LiveDesign

In my LiveDesign

- Simple Glide docking
- Or more complex workflow (eg ensemble docking...) see the workflow examples

KNIME workflow run in LiveDesign – Structure rendering

DATA & COLUMNS

Project LiveReport

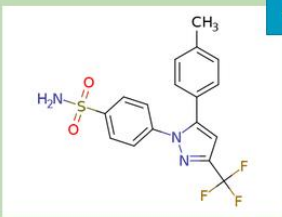

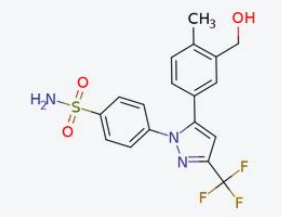

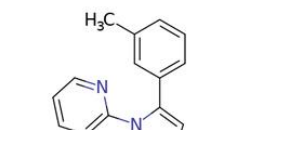

Search columns

KNIME

Aniline Genotoxicity (Energy...)

- Docking
- Docking and protein surf...
- Docking and protein surf...
- Docking and rendering_
- Docking_
- DockingWithSurfaces
- DockingWithSurfaces-Mac
- DockingWithSurfaces-Mac2
- Ensemble docking
- Installation test
- LD docking
- Property radar plot (volume)
- PropertyRadarPlotModel
- PropertyRadarPlotModel...
- Protonation forms

Open Live Report + Reception Review copy

| | Compound Structure | ID | Docking and rendering_ (3D) | Docking and rendering_ (docking score) |
|---|--|------------|--|--|
| 1 |  | CMPD-10409 |  | -5.3 |
| 2 |  | V58164 |  | -5.4 |
| 3 |  | V64836 |  | |

Atom selection

res.num 109, 168, 53

OK Apply Cancel ?

VISUALIZE + 3D

Contents

- COX1 (3D)
- COX2 (3D)
- Docking (3D)
- Docking and protein ...
- Docking and protein ...
- ☒ Docking and renderin...
- ☒ protein
- ☒ CMPD-10409
- + 1 pose
- DockingWithSurface...
- Docking_ (3D)
- Ensemble docking (3D)

+

Add 3D models to visualize selected compounds: Click here, then browse or search for any models containing the word '(3D)' in the list that appears on the left.

Glide Grid Reader

SDF Reader

Compound structures from the LiveReport

Save in the workflow

LigPrep

Generate 3D coordinates

Glide Ligand Docking

Extract Properties

Title

Row Splitter

No protein

Display

Binding site only

Residue information

Important ones

Representation

Important ones in ball and stick

Concatenate

Column Filter

Only relevant columns for the Live Report

Save Workflow

Before exporting to LiveDesign

CASE Switch Data (Start)

Credentials Configuration

LiveDesign

Upload model to LiveDesign

In my LiveDesign

KNIME workflow run in LiveDesign – Protein surface

8

DATA & COLUMNS

Project LiveReport

Search columns

KNIME

Aniline Genotoxicity (Energ...

Docking

Docking and protein surf...

Docking and protein surf...

Docking and rendering_

Docking TMP

Docking_

DockingWithSurfaces

DockingWithSurfaces-Mac

DockingWithSurfaces-Mac2

Ensemble docking

Installation test

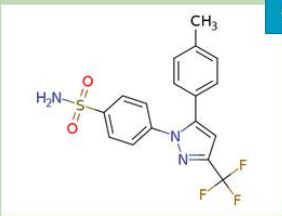

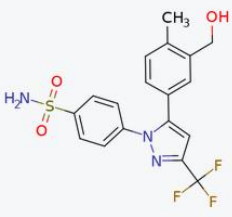

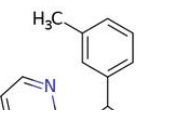

LD docking

Property radar plot (volume)

PropertyRadarPlotModel

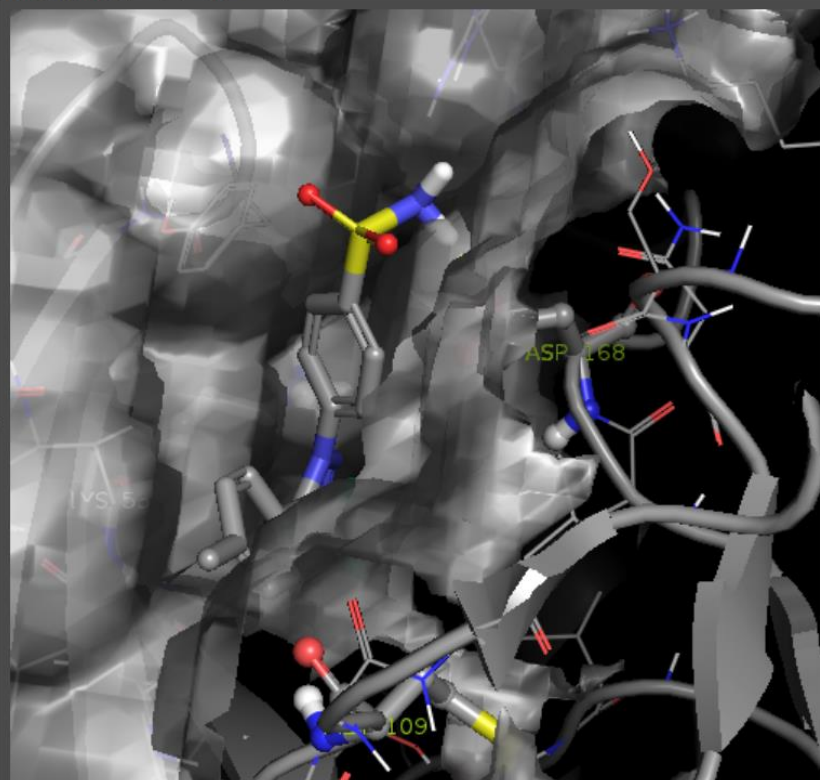
Open Live Report

Reception Review copy

| | Compound Structure | ID | Docking and protein surface_ (3D) | Docking and protein surface_ (docking score) |
|---|---|------------|--|--|
| 1 |  | CMPD-10409 |  | -5.3 |
| 2 |  | V58164 |  | -5.4 |
| |  | V64836 |  | -5.3 |

VISUALIZE +

3D



Contents

Styles

☐ COX1 (3D)
☐ COX2 (3D)
☐ Docking (3D)
☐ Docking and protein sur
☒ Docking and protein sur
☒ protein
☒ CMPD-10409

+ 1 pose

☐ DockingWithSurfaces (3
☐ Docking_ (3D)
☐ Ensemble docking (3D)
☐ LD docking (3D)

+

Add 3D models to visualize selected compounds: Click here, then browse or search for any models containing the word '(3D)'

Glide Grid Reader

SDF Reader

Saved in the workflow

LigPrep

Generate 3D coordinates

Glide Ligand Docking

Sitemap surface

Extract Properties

Row Splitter

Display

Residue information

Representation

Concatenate

Run Maestro

Rendering checking

Cross Joiner

Column Filter

Only relevant columns for the Live Report

Save Workflow

CASE Switch Data (Start)

Credentials Configuration

Upload model to LiveDesign

In my LiveDesign

Binding site only

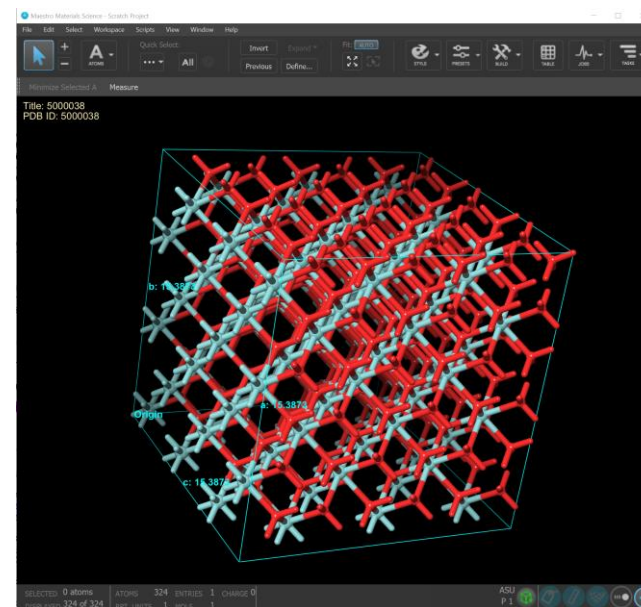
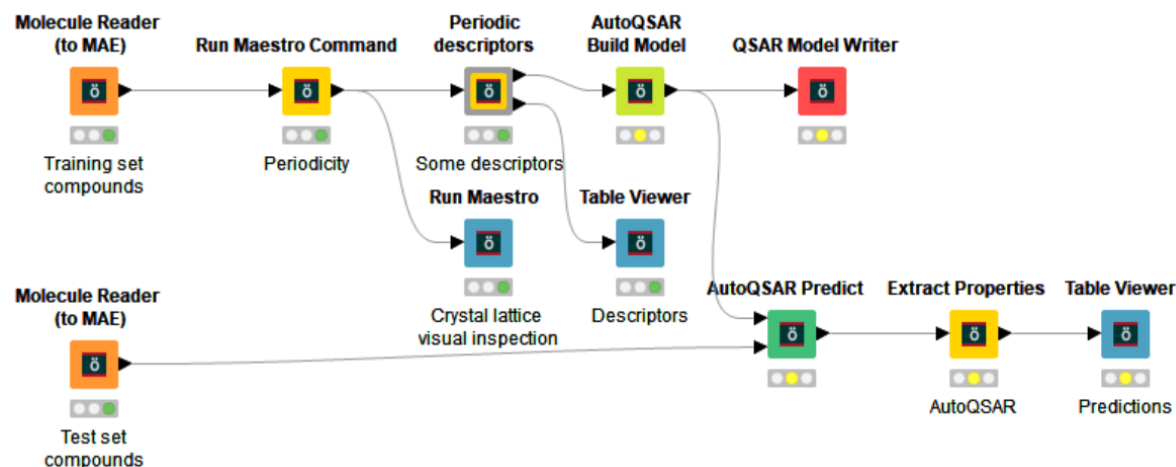
Important ones

Important ones in ball and stick

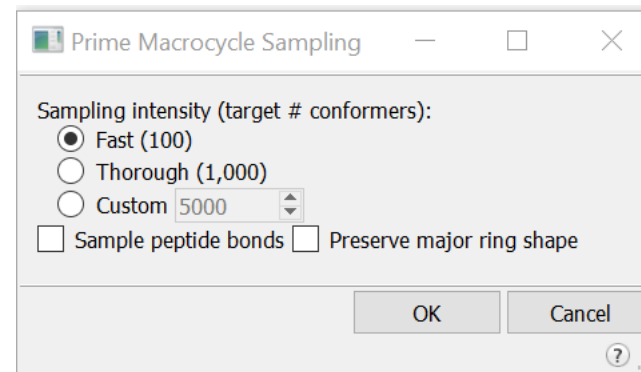
Before exporting to LiveDesign

Other new features and nodes

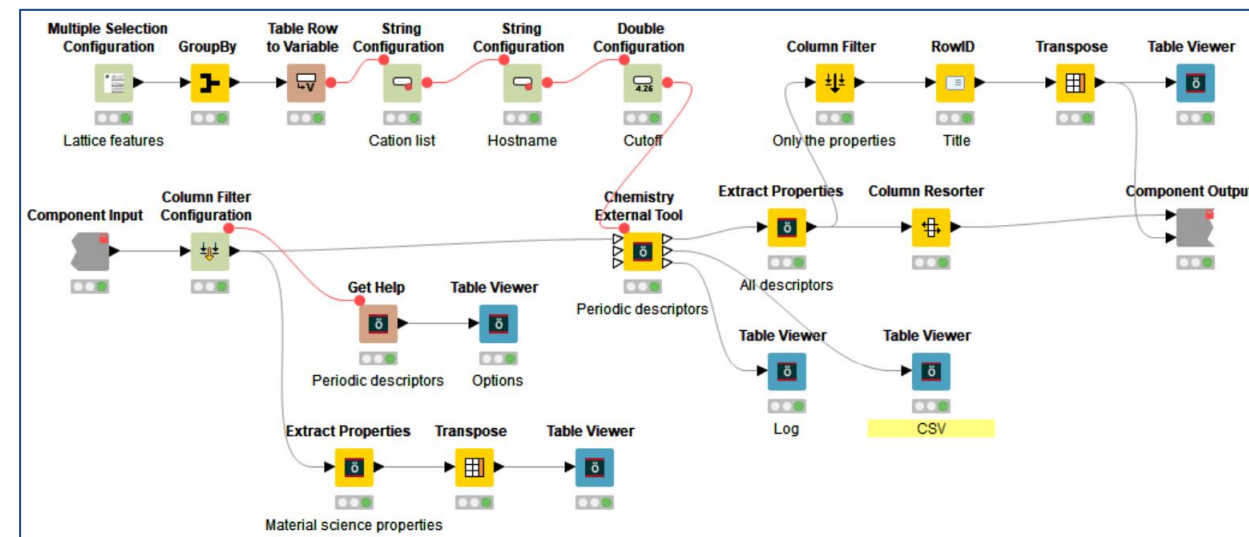
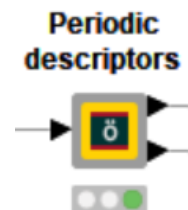
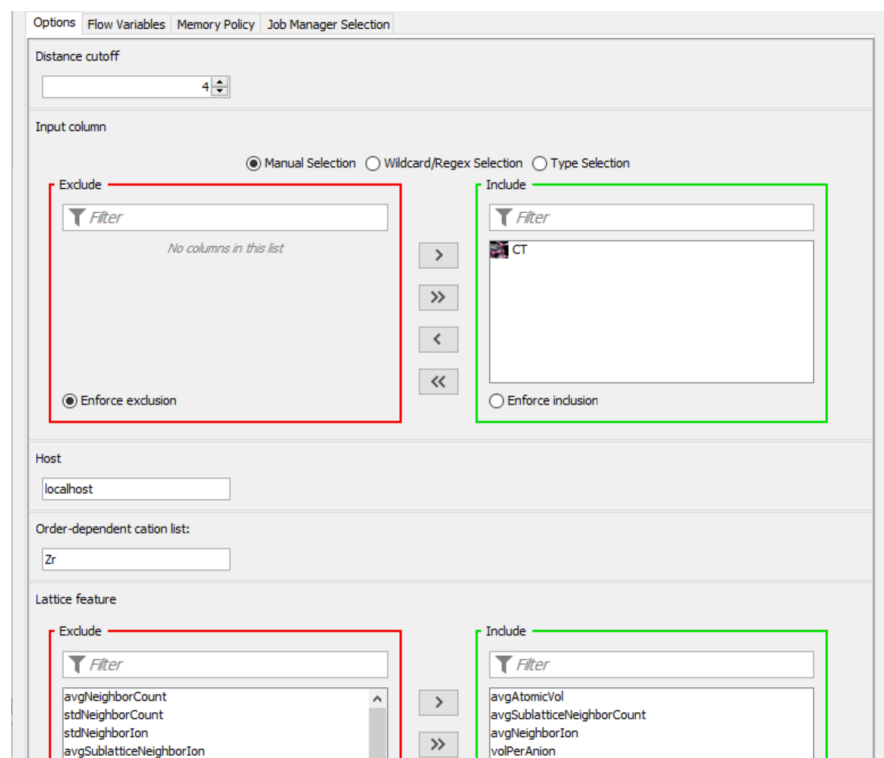
- The Molecule reader node takes in cif format



- New Prime Macrocycle Conformation sampling node
- Some Components
 - Look and feel like real nodes
 - Searchable and available from the KNIME hub website
 - Drag and drop from the hub page
 - Not in the node repository, but available in between releases



Components on the KNIME hub



- The Schrodinger workflow examples are available on the KNIME hub https://hub.knime.com/schroedinger/spaces/Workflow_examples/latest/
- The Schrodinger nodes are searchable from the KNIME hub
 - And the workflows using a specific node are listed

Components and Workflow Examples

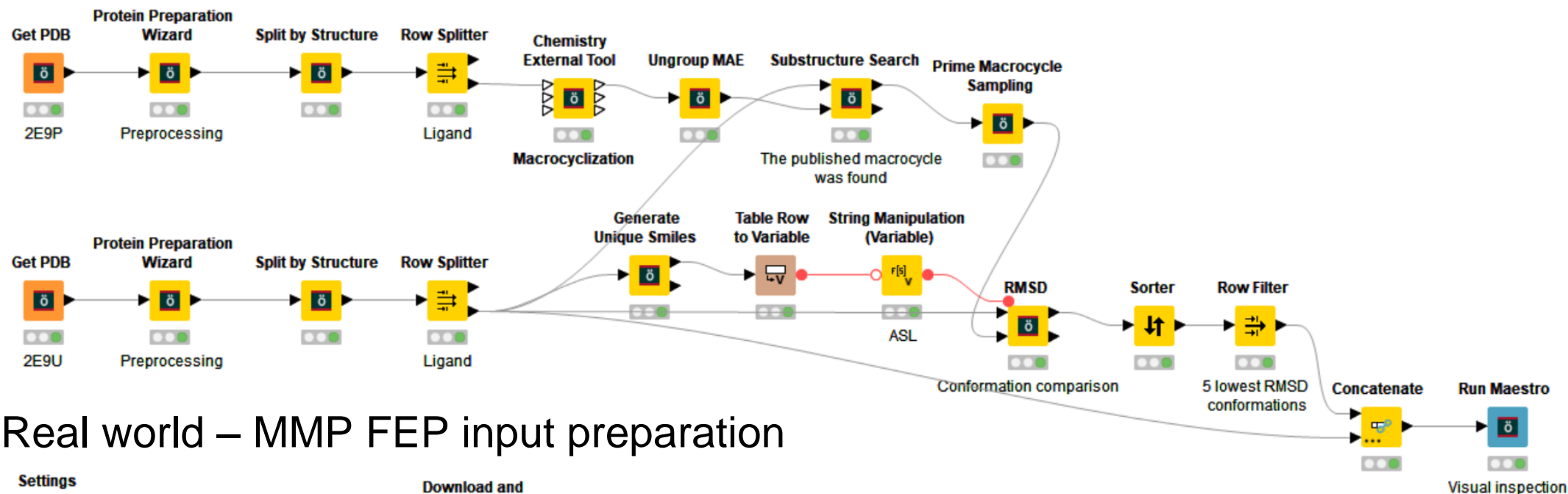
- **Components**
 - Membrane permeability
 - Periodic descriptors
 - Rendering: Atom representation, Display atoms, Residue information label
 - Sequence converter, Excel to fasta
 - Job control
- **Workflows to be run in LiveDesign**
 - Docking, including a customized rendering of the binding site
 - Docking and protein surface
 - Ligand ESP surface
 - Ligand property radar plot
 - Low energy conformation
 - Example running on a KNIME server
- **LiveDesign – Import and export**
 - A radar plot and 2D structure are added to the LiveReport as image columns
- **Docking in the most similar binding site**
- **ADME – Physics-based Membrane Permeability**
- **Material Science – Periodic descriptors**
- **Tools – Debugging workflow**
 - To help diagnosis installation and execution failures
- **Workbench – Text cell parsing**

Available on:

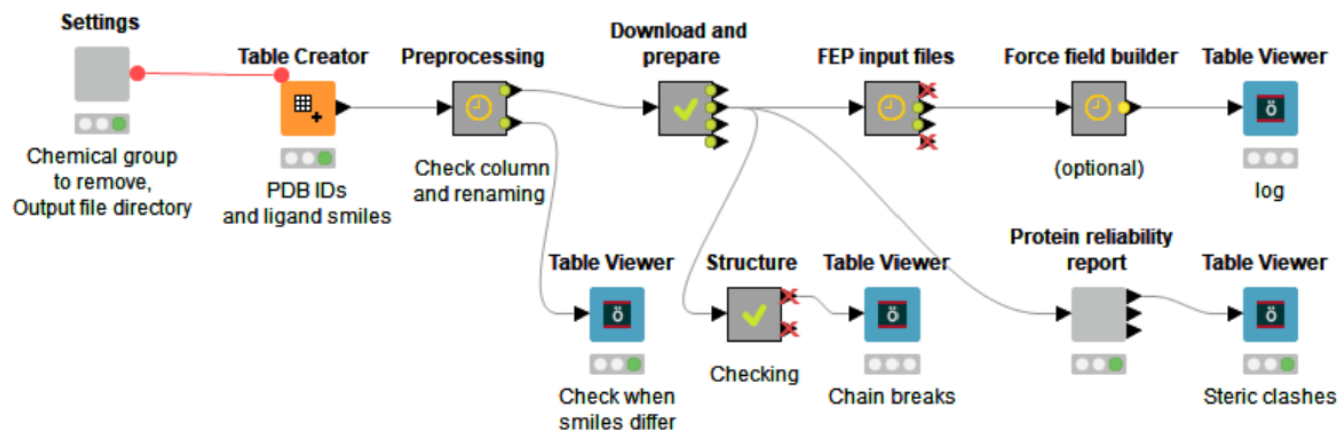
https://hub.knime.com/schroedinger/spaces/Workflow_examples/latest/

Workflow Examples

- Molecular Mechanics – Macrocyclization and macrocycle conformational search



- Real world – MMP FEP input preparation





New features in the KNIME extension

In Schrödinger Suite 2020-1

2020-1 New Features

- Includes the latest version of KNIME (v4.1)
- New node to upload workflows **from a KNIME server to be run from LiveDesign**
- Usability improvements of the Upload model to LiveDesign node
- New Export image to LiveDesign node
- **Export to LiveDesign** node can create an extra **molecule column**
- Job information for failing calculation diagnostics
- The reader nodes keep the navigation history

KNIME Analytics Platform 4.1 - some new features

See details on <https://www.knime.com/whats-new-in-knime-41>

KNIME Hub - Private & Public Spaces Access to Components

KNIME Analytics Platform

- **Navigation in the Workflow Canvas**
 - Ctrl-F to search for nodes by name, ID, or description in a workflow
 - Most recently opened workflows in your workspace.
- **Machine Learning and Guided Labeling**
Binary Classification Inspector node. Active Learning and Weak supervision
- **Components**
 - Editing a shared component on the KNIME Hub or your local workspace by double clicking the component.
 - Component Description view
- **New nodes**
 - Row Filter (Labs) to filter rows based on complex queries comprising conditions on multiple columns - including the row index and row ID. Webpage Retriever
 - Top k Selector
- **Big Data** - Databricks, Google Cloud and Apache Knox Support
- **KNIME Database Extension** - Migration to the new DB

framework. New DB Connection Extractor and Closer node.

- **Partner Extensions** Privacy Nodes to anonymize data
- **Technical Improvements**
 - **Dynamic Ports** : add and remove ports to some nodes (those with three black dots in the bottom left corner eg the Concatenate node)
 - **New Flow Variable Types** : New boolean, long, and array types e.g. filtering a number of columns is possible using an array variable.

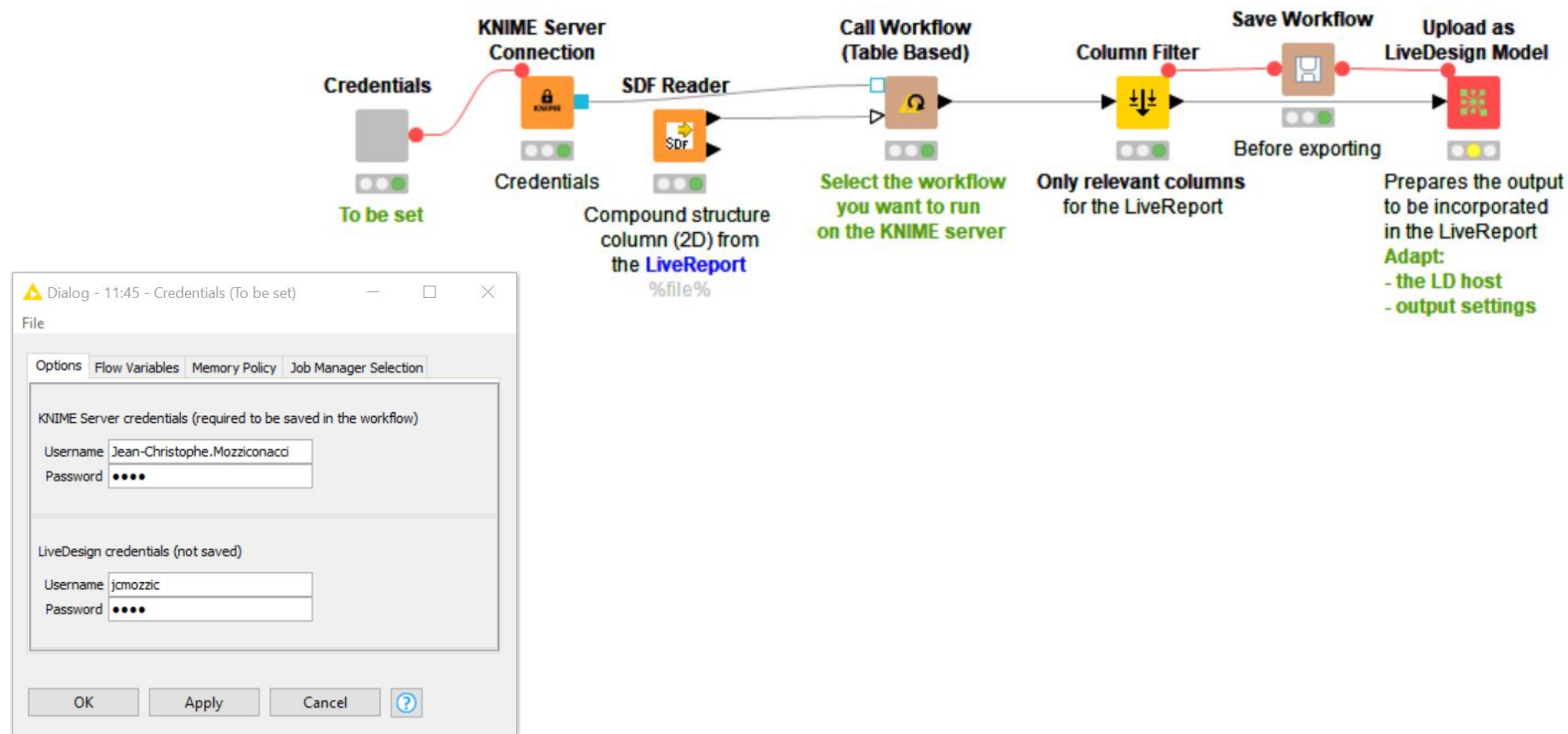
KNIME Server 4.10

- **Configuration Dialog**
Pass configurations to a job when executing or for running on a schedule
- **Call Workflow Action**
 - Call (possibly conditionally) one or more new workflows once the current workflow is finished
- **Enterprise Features**
 - OAuth/OpenID Connect
 - **Server Managed Customization Improvements**
Host update sites in your own network if you are unable to connect directly to our own update sites due to proxy restrictions.

Run a workflow on a KNIME Server from LiveDesign

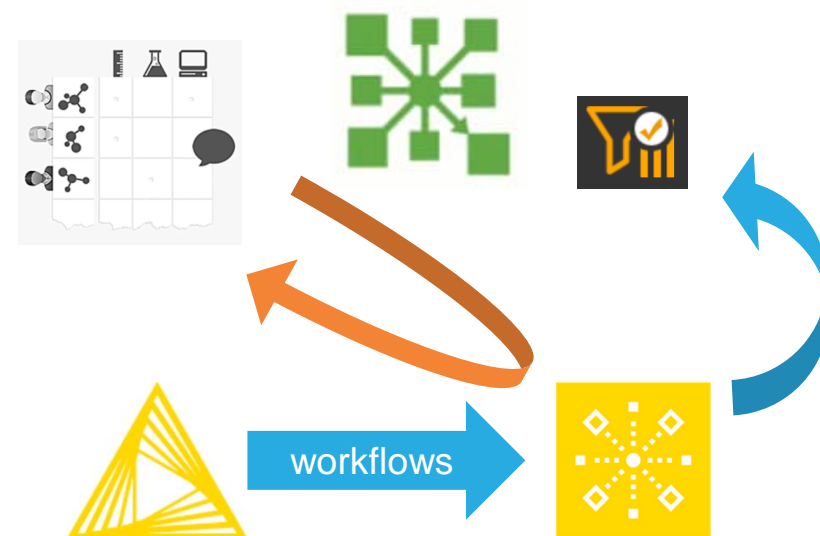
- Simply using the Upload as LiveDesign model node

<https://kni.me/w/R0pmPpC2gs9FSyCU>



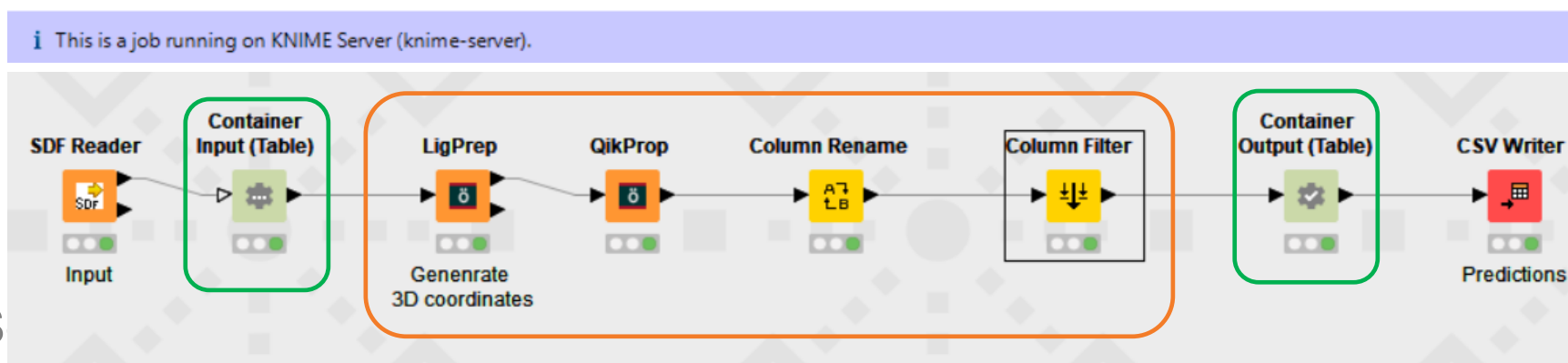
Upload workflows from a KNIME Server and to be run in LiveDesign

- Upload to LiveDesign all the workflows stored in a group on a KNIME Server
 - The new or updated workflows on the KNIME server are accessible as Computational models in LiveDesign
- When invoking these Computational models in LiveDesign the workflows are run on the KNIME server
 - The data is copied back from the KNIME server to populate the LiveReport
 - The computation resources of the KNIME server are used
 - And the KNIME installation (extensions) on the KNIME server
 - Instead of the installation on the LiveDesign instance



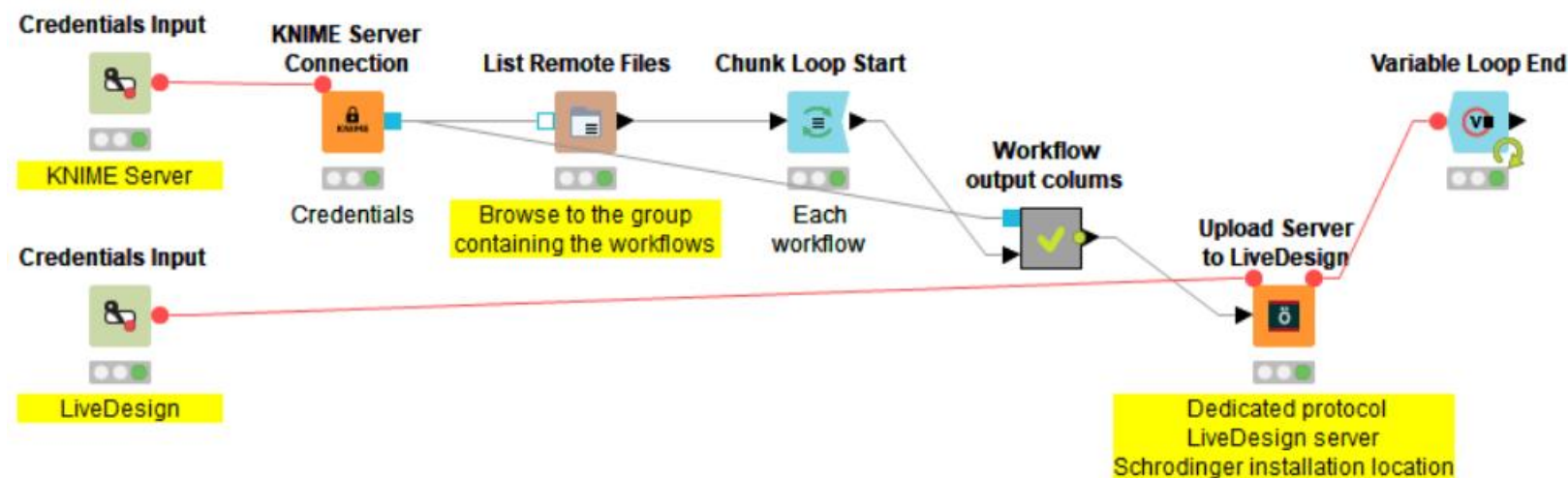
Requirements

- A dedicated LiveDesign protocol
 - To create the Computation models corresponding to the KNIME server workflows
 - It stores credentials to access to the KNIME and LiveDesign servers
 - Ask your Solution Architect to add it
- KNIME server workflows to be invoked in LiveDesign
 - Must include the Container input and output nodes
 - The Container nodes can't handle Maestro columns for now



Upload workflows to be run on a KNIME Server

- Workflow to upload or update KNIME server workflows in LiveDesign
 - It can be run manually from a KNIME client when new workflows are added to the KNIME server
 - Or run as a scheduled task on the KNIME server
 - And use the KNIME server credentials
 - It configures the corresponding LiveDesign Computational models to run these workflows on the KNIME server



Upload model to LiveDesign node – Overview image

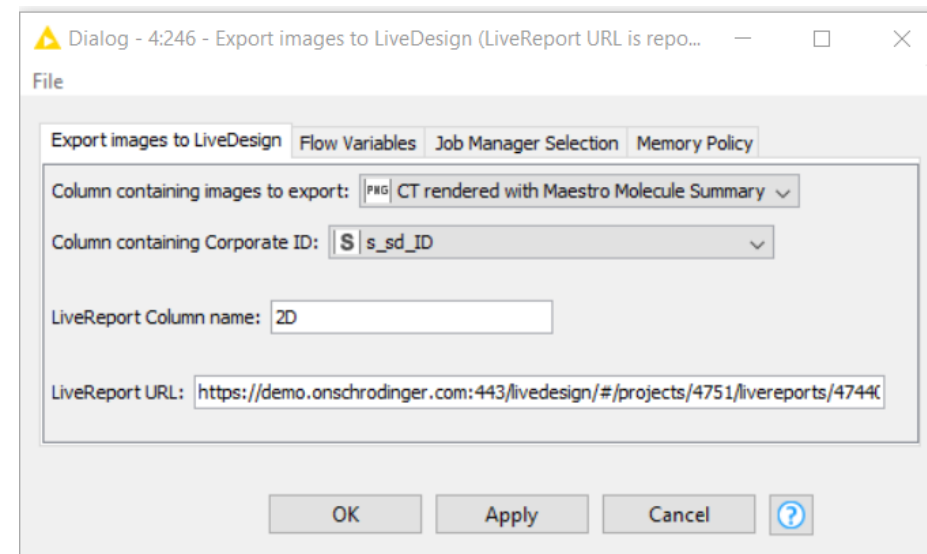
- The workflow overview can be inspected directly from the Task page on LiveDesign Admin panel <https://LiveDesignServer.com/admin/tetasks/task/>

The screenshot displays the 'LiveDesign Admin' interface. At the top, a green header contains the 'LiveDesign Admin' logo and a breadcrumb trail: 'Home > Tasks > 5e1b7ea0757a47fe04f8575d'. Below this, the 'Task Details' section shows the task ID '5e1b7ea0757a47fe04f8575d', its status as 'Finished', and the submitter 'jean'. A dropdown menu for 'Input files:' is open, listing four files: 'LiveDesign - KNIME_server_execution.knwf (download)', 'workflow.svg (download)' (which is circled in red), 'params.json (download)', and 'input.sdf (download)'. To the right of the dropdown, a workflow diagram is shown, starting with an 'SDF Reader' node, followed by 'LigPrep', 'QikProp', 'Extract Properties', 'Model Reader', 'Random Forest Predictor (Regression)', 'Column Filter', 'Credentials Input', and finally 'Upload model to LiveDesign'. Each node has a brief description of its function.

- And the node is more robust and has other usability improvements

Export to LiveDesign nodes

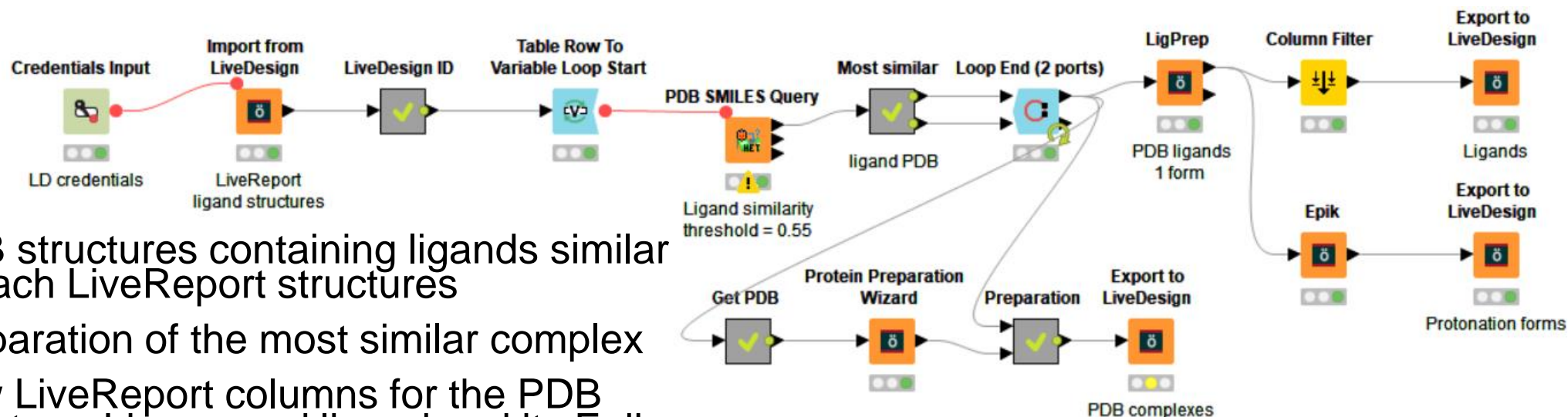
- Export image to LiveDesign node
 - To export PNG images (eg 2D molecule view, plots, Ligand interaction diagram...)
 - The LiveReport URL from LiveDesign web interface or reported by the Import and export nodes in the console
- Create an extra molecule column with the Export to LiveDesign node
 - To store ligand conformations, docking poses, PDB complexes...

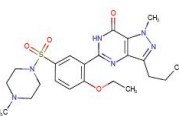





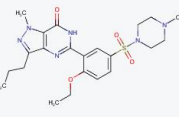








| Compound Structure | ID | Docking complexes (3D) | Docking poses (3D) | 2D view | PDB ligand (3D) | Epik (3D) | PDB (prepared with version) | PDB (PDB ID) | PDB (3D) |
|--------------------|------------|------------------------|--------------------|---------|-----------------|-----------|-----------------------------|--------------|----------|
| | CHEMBL192 | | | | | | 2020-1 2020-1 | 1TBF 1TBF | |
| | CMPD-10182 | | | | | | 2020-1 2020-1 | 1TBF 1TBF | |

Export to LiveDesign – structure columns

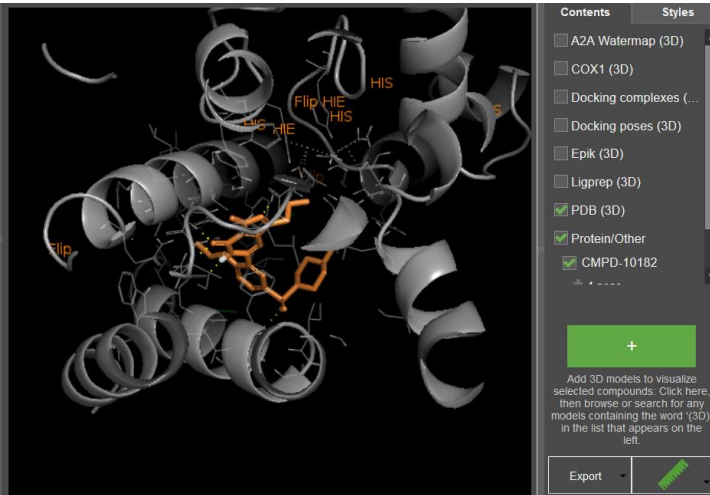
- PDB structures containing ligands similar to each LiveReport structures
- Preparation of the most similar complex
- New LiveReport columns for the PDB structure, Ligprepped ligand and its Epik protonation forms.



| Compound Structure | ID | Docking complexes (3D) | Docking poses (3D) | 2D view | PDB ligand (3D) | Epik (3D) | PDB (prepared with version) | PDB (PDB ID) | PDB (3D) |
|---|------------|---|---|---|---|---|-----------------------------|--------------|---|
|  | CHEMBL192 |  |  | |  |  | 2020-1 2020-1 | 1TBF 1TBF |  |
|  | CMPD-10182 |  |  |  |  |  | 2020-1 2020-1 | 1TBF 1TBF |  |

10 Compounds • 1 Selected 32 Columns (4 Hidden)

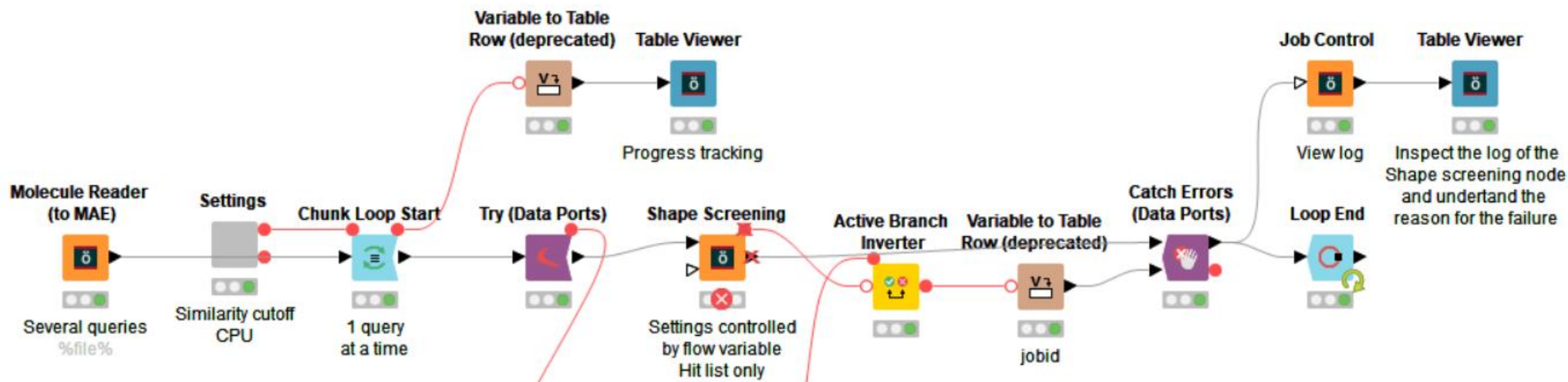
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The 3D visualization shows a protein structure with a ligand bound in the active site. The sidebar on the right lists the contents and styles of the visualization, including A2A Watermap (3D), COX1 (3D), Docking complexes (3D), Docking poses (3D), Epik (3D), Ligprep (3D), PDB (3D), Protein/Other, and CMPD-10182. The 'PDB (3D)' and 'Protein/Other' options are checked. The 'Export' button is visible at the bottom right.

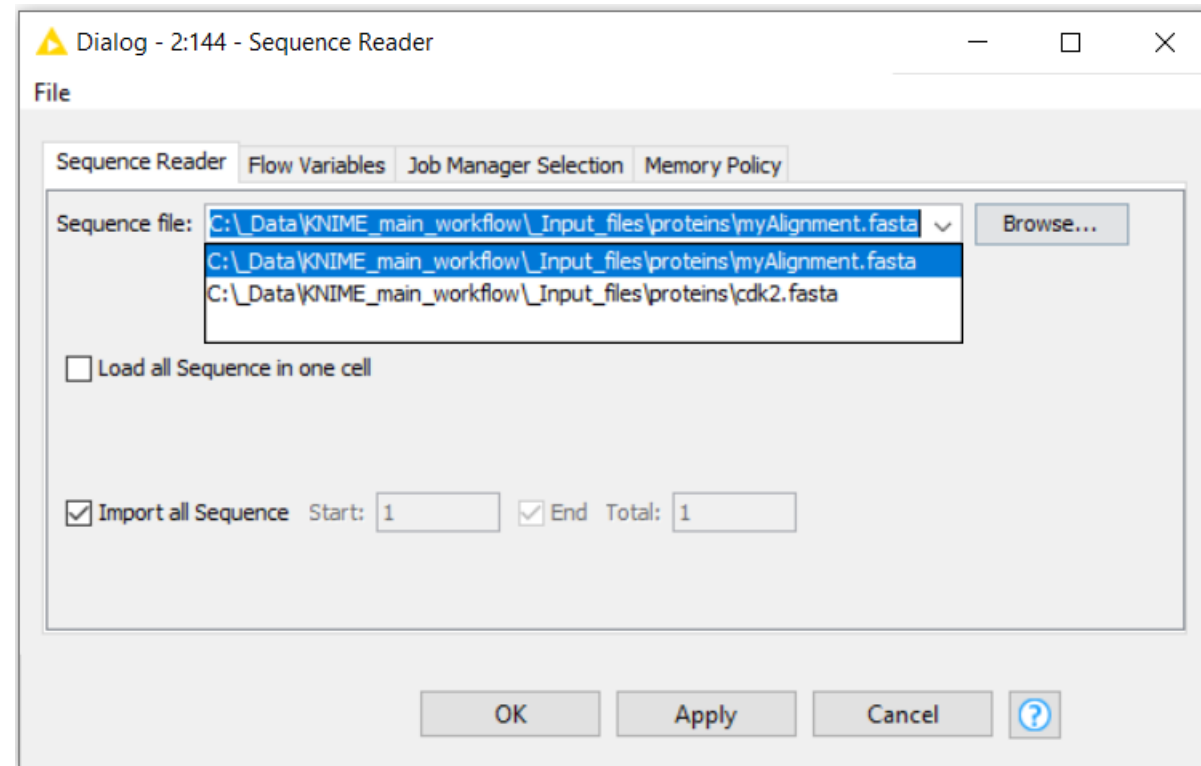
Diagnose more easily failing calculations

- The Job control ID is stored as flow variable
 - Even if the node failed
- As input for the Job control node
 - Display the status, error message, log file...
 - Key on a KNIME server when the node view can't be inspected



Reader nodes – navigation history

- The default location is your home directory for new nodes
- The reader nodes point to the location of the last opened file when reopening
- The recently opened files are listed in the single file reader nodes
- And other robustness improvements
- The Structure filter node smiles/smart filter file option takes URLs
 - Can point to a file embedded in the workflow



- String and numeric values can be passed when executing a workflow in batch
 - Application example: pass a file path
- Label Configuration or Quick from nodes with %input%
- In the KNIME_batch.py invocation -i<var_name>
 - eg \$SCHRODINGER/run KNIME_batch.py \${workflow:FILE-INPUT} -workflow_path "\${workflowPath:TEXT-INPUT}" -run -debug -isdf \${SDF-FILE} ...
 - See details in KNIME_batch.py -printallowed output

New and Improved Workflow Examples

- **LiveDesign – Upload from KNIME server**
 - Upload a group of workflows from the server
 - A couple of workflows ready to be uploaded to be executed on the KNIME server from LiveDesign
- **LiveDesign – Upload as computational models**
 - Schrodinger/KNIME installation check
 - Align LiveReport ligands on a reference ligand using Shape screening
 - Replace functional groups of each LiveReport ligand with bioisosteres, generating all the single replacements
- **LiveDesign – Import and export**
 - Export images of the molecule 2D rendering
 - Find related PDB structures
- **Server setup diagnosis**
- **Pharmacophore – Shape**
 - Investigate calculation failures with the Job control node
- **Tools – Job control**
 - Component with comprehensive output



New features in the KNIME extension

In Schrödinger Suite 2019-4

2019-4 New Features

- Includes the latest version of KNIME (v4.0.1)
- New **Batch test** node
- The FEP+ reader node reports health information and representative structures
- The **Upload model to LiveDesign node can update an existing model** and supports workflows **with molecule output**
- The KNIME-Maestro connector node runs in batch

Batch test node

- Add the node to your workflow and execute it

The workflow is run in batch using KNIME_batch.py. This script has been in place for years and is used to run KNIME workflows in Maestro for instance.

- The command line to run, the execution directory, time and other available options to consider using are reported in the output table
- The temporary files aren't removed if the execution fails
So they can be inspected for debugging purpose
- The calculation progress can be tracked in the Log view

The screenshot displays two windows from the KNIME software. The top window, titled 'Table View - 2:15227 - Table Viewer (Command run)', shows a table with four columns: 'Row ID', 'KNIME_batch command', 'Job Directory', and 'Job Info'. The first row (Row0) contains the following data:

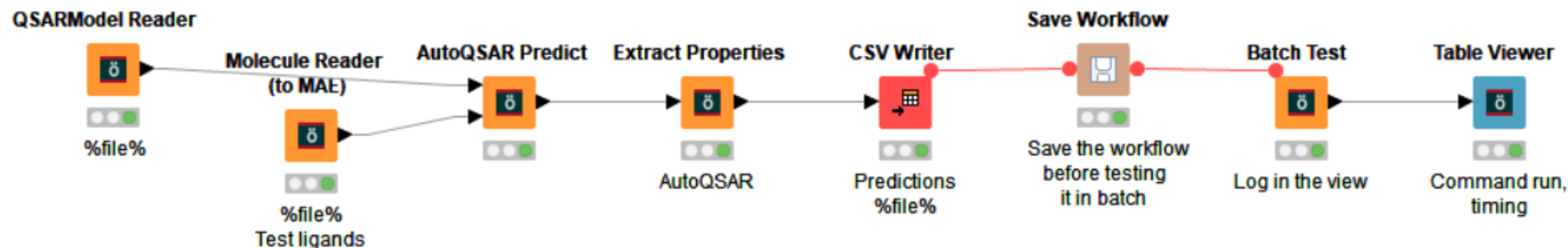
| Row ID | KNIME_batch command | Job Directory | Job Info |
|--------|--|---|---|
| Row0 | \$SCHRODINGER/run KNIME_batch.py "C:\Users\jcmozzic\AppData\Local\Temp\BatchTest_15011..." | C:\Users\jcmozzic\AppData\Local\Temp\BatchTest_1501135287 | SCHRODINGER = C:/Program Files/Schrodinger2019-4 Time taken to execute the workflow in batch = 153.073 seconds |

The bottom window, titled 'knime.log - 2:29 - Batch Test (Log in the view)', shows a log of debug and info messages. The log indicates that the workflow did not execute successfully. Key messages include:

- DEBUG : main : MAEMultiFileReaderNodeModel : Molecule Reader (to MAE) : 0:9 : Removing all (0) views from ^
- DEBUG : main : Node : Molecule Reader (to MAE) : 0:9 : clean output ports.
- DEBUG : KNIME-Temp-File-Deleter : Buffer : : Deleted temporary file "C:\Users\jcmozzic\AppData\Local\
- DEBUG : main : AbstractTableStoreReader : Molecule Reader (to MAE) : 0:9 : Closing input stream on "C:\Us
- DEBUG : main : WorkflowManager : : : Project "Batch execution NEW 0" removed (1 remaining)
- DEBUG : main : NodeContainer : : : ROOT has new state: EXECUTED
- INFO : main : BatchExecutor : : : ===== Workflow did not execute successfully =====
- DEBUG : KNIME-Temp-File-Deleter : Buffer : : Deleted temporary directory "C:\Users\jcmozzic\AppData\I
- DEBUG : KNIME-Temp-File-Deleter : Buffer : : Deleted temporary file "C:\Users\jcmozzic\AppData\Local\

Batch test node – Applications



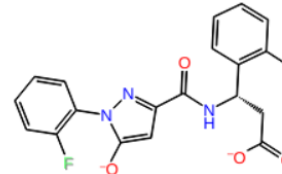

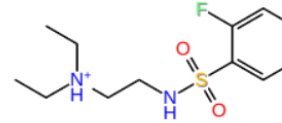


- **Frame the command to execute the workflow through the command line**
 - Based on the reader and writer nodes tagged with %file%
- **Check the workflow runs fine in batch**
 - Before uploading it to LiveDesign or running it on a remote machine.
This is especially convenient when working on Windows
 - Test and choose execution options
 - If it fails you can share the workflow including the batch node
It will help our support team or a colleague to investigate the problem



| | |
|--------|--|
| Row ID | S KNIME_batch command |
| Row0 | \$SCHRODINGER/run KNIME_batch.py "C:\tmp\KNIME\Schrodinger\BatchTest_74391943\Batch_execution.knwf" -run -istruct knime://knime.workflow/input/ligs.mae -iqzip knime://knime.workflow/input/AutoQSARmodel.qzip -otxt /tmp/predictions. |
| | J Job Directory |
| | -data C:\tmp\KNIME\Schrodinger\BatchTest_74391943\workspace -destFile=C:\tmp\KNIME\Schrodinger\BatchTest_74391943\Batch_execution-executed.knwf -reset -suppressErrors C:\tmp\KNIME\Schrodinger\BatchTest_74391943 |

FEP+ Reader - improvements

- Extracts information from a set of fmp files
 - Same information as in Maestro FEP panel tabs:
 - Overview
 - Analysis
 - Includes representative lambda 0 and 1 frames
 - Optionally extracts the trajectories to inspect other frames
 - Health information

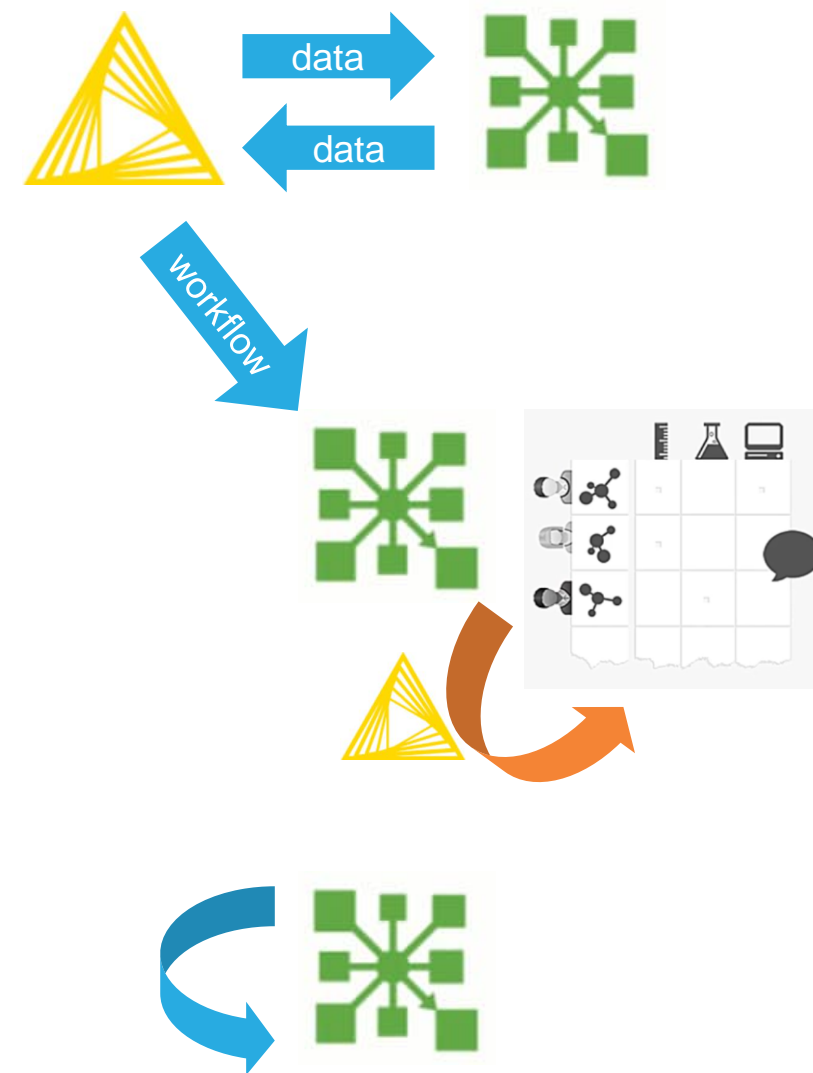
| Row ID | S Filename | S Ligand | D Pred. dG | D Pred Error | SM Structure |
|--------|----------------------|----------|------------|--------------|---|
| Row56 | fep_F-H_3UVP_out.fmp | 3UVP_PDB | 0 | 0.4 |  |
| Row58 | fep_F-H_3ZC6_out.fmp | 3ZC6_PDB | 0 | 0.4 |  |
| Row60 | fep_F-H_4AZ0_out.fmp | 4AZ0_PDB | 0 | 0.4 |  |
| Row63 | fep_F-H_4B80_out.fmp | 4B80_PDB | -0.7 | 0.41 |  |
| Row65 | fep_F-H_4B82_out.fmp | 4B82_PDB | 0.38 | 0.41 |  |
| Row67 | fep_F-H_4BCD_out.fmp | 4BCD_PDB | -0.35 | 0.41 |  |
| Row68 | fep_F-H_4CSJ_out.fmp | 4CSJ_PDB | 0 | 0.4 |  |

| S Filename | S Receptor Health | S Ligand Health | S FMPdb... |
|-----------------------|---|---|------------|
| fep_F-H_1BZH_out.fmp | "Potential receptor issues: 2 buried unsatisfied donor, 2 waters with no hb partners, 13 backbone dihedrals, 17 unusual b-factors, 3 peptide planarity" | 2 ligands have Missing torsion parameters | OK |
| fep_F-H_vacuum_1BZ... | "Potential receptor issues: 2 buried unsatisfied donor, 2 waters with no hb partners, 13 backbone dihedrals, 17 unusual b-factors, 3 peptide planarity" | 2 ligands have Missing torsion parameters | OK |
| fep_F-H_1BZH_vacuu... | "Potential receptor issues: 5 waters with no hb partners, 2 unusual b-factors, 8 peptide planarity" | 2 ligands have Missing torsion parameters | OK |
| fep_F-H_1D3G_out.fmp | "Potential receptor issues: 5 waters with no hb partners, 2 unusual b-factors, 8 peptide planarity" | 2 ligands have Missing torsion parameters | OK |
| fep_F-H_1d3g_mod_o... | "Potential receptor issues: 5 waters with no hb partners, 2 unusual b-factors, 8 peptide planarity" | 2 ligands have Missing torsion parameters | OK |
| fep_F-H_vacuum_1D3... | "Potential receptor issues: 5 waters with no hb partners, 2 unusual b-factors, 8 peptide planarity" | 2 ligands have Missing torsion parameters | OK |
| fep_F-H_1GSZ_out.fmp | "Potential receptor issues: 2 buried unsatisfied donor, 3 buried unsatisfied acceptor" | 1 ligand has Missing torsion parameters | OK |
| fep_F-H_vacuum_1GS... | "Potential receptor issues: 2 buried unsatisfied donor, 3 buried unsatisfied acceptor" | 1 ligand has Missing torsion parameters | OK |

- Typical applications: merge, filter, triage, tag and analysis of multiple single edge FEP runs

LiveDesign Nodes in KNIME

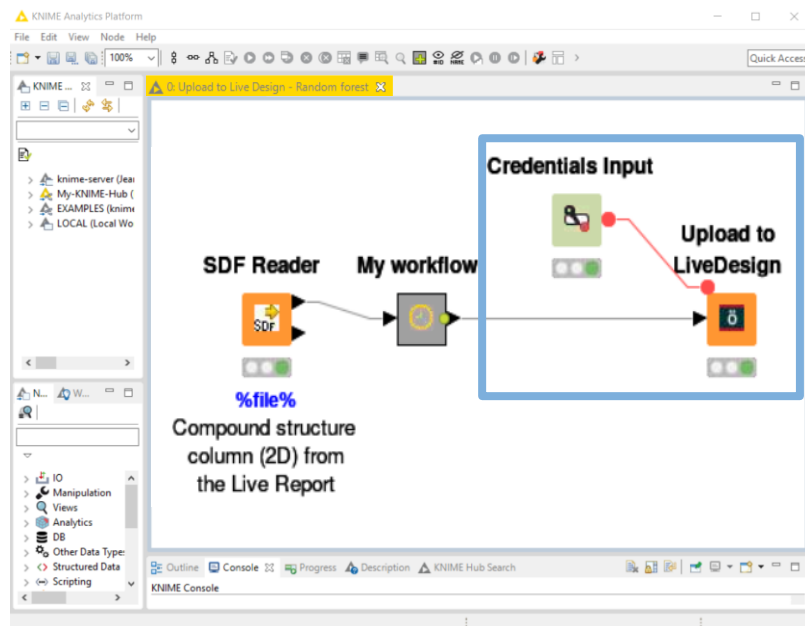
- **Import from LiveDesign**
 - Populates a KNIME table with data from a LiveReport
- **Export to LiveDesign**
 - Sends data from a KNIME table to a LiveReport
- **Export images to LiveDesign**
 - PNG or SVG images stored in Free Form Columns
- **Upload a workflow as LiveDesign model**
 - Creates a model which executes the KNIME workflow in LiveDesign
(no need to open the LiveDesign administration panel)
 - The model is now ready to be run on any LiveReport and the output will be added as new column(s)
- **Administrate LiveDesign models and protocols**
 - eg backup copies, testing copies, copy from testing to production instance, new version deployment, version comparison



Upload a workflow to LiveDesign Node

- In the workflow in KNIME
 - Label the SDF reader node
 - Execute the Upload model to LiveDesign node

The workflow is uploaded to LiveDesign as Model and available under Computational



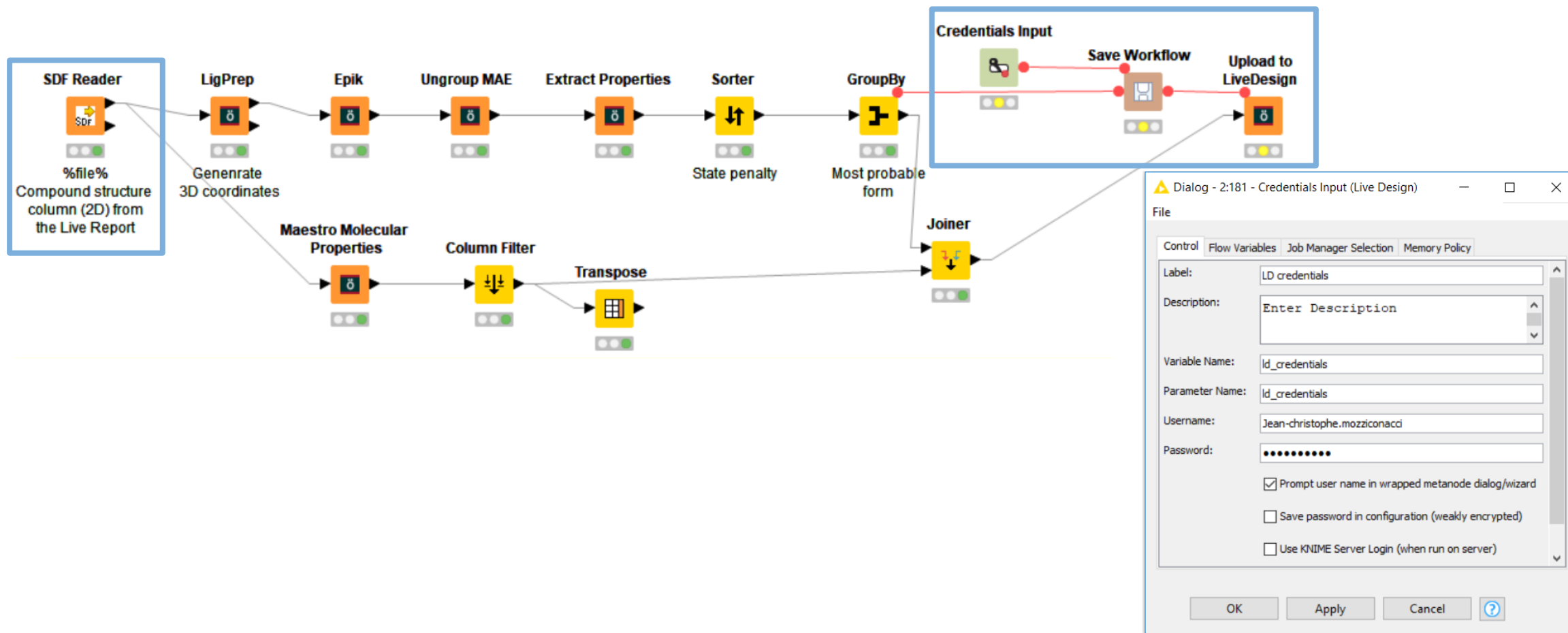
models > KNIME section in LiveDesign.

- In the LiveReport
 - The KNIME workflow is run on the LiveReport compound structures and new column(s) added

| | Compound Structure | ID | All IDs | 3D (3D) | Upload to Live Design (Extensions) | 19-3 KNIME QSAR (Prediction) |
|---|--------------------|--------|---------|---------|------------------------------------|------------------------------|
| 1 | | V35000 | V35000 | | | 23 |
| 2 | | V35002 | V35002 | | | 27 |
| 3 | | V35006 | V35006 | | | 5 |
| 4 | | V35010 | V35010 | | | 19 |

Upload a workflow to LiveDesign – in KNIME

- Any workflow with a tagged input SDF reader node and text/numeric or Maestro output columns passed to the Upload to LD node



Upload a workflow to LiveDesign – in LiveDesign

- The workflow is uploaded as Model to LiveDesign

- Using dedicated KNIME protocols

- Ask your Solution Architect to add the generic one to your LiveDesign instance

- The workflow is run on the LiveReport structures using KNIME_batch.py and new columns added

The screenshot displays the LiveDesign interface. On the left, the 'DATA & COLUMNS' sidebar shows a tree view of workflows. The 'KNIME' folder is highlighted with a red circle, containing sub-items like 'Upload to Live Design' and 'Upload to Live Design - Random forest'. The main table lists chemical structures with their IDs and associated data. The 'Upload to Live Design (Extensions)' and 'Upload to Live Design (Test)' buttons are circled in red.

| | Compound Structure | ID | All IDs | 3D (3D) | Upload to Live Design (Extensions) | Upload to Live Design (Test) |
|---|--------------------|--------|---------|---------|------------------------------------|------------------------------|
| 1 | | V35000 | V35000 | | | |
| 2 | | V35002 | V35002 | | | |
| 3 | | V35006 | V35006 | | | |
| 4 | | V35010 | V35010 | | | |

Upload to model LiveDesign – Improvements

Fields to specify:

- The LiveDesign instance
- The LiveDesign protocol
 - The generic protocol
“KNIME workflow 19-4” protocol is compatible with the new version of the node
 - Modified protocols can be used for specific scenarios. To be added using LiveDesign Admin page.
- The Schrodinger installation version
 - Running the same KNIME version as used to create the workflow
 - The default is used if empty
- Overwrite model
 - To update an existing model
- Corporate ID column
 - Column to be used to match the workflow results with the LiveReport entries

The screenshot shows a dialog box titled 'Upload to LiveDesign' with three tabs: 'Job Manager Selection', 'Memory Policy', and 'Flow Variables'. The 'Job Manager Selection' tab is active. Inside the dialog, there are several input fields and a checkbox:

- LiveDesign host:** A text field containing 'https://demo.schrodinger.com'.
- LiveDesign protocol:** A dropdown menu showing 'KNIME Workflow 19-4 (2062)' with a 'Refresh' button to its right.
- Schrodinger Suite:** An empty text field.
- Corporate ID column:** A dropdown menu showing 'Molecule name'.
- Overwrite model:** A checked checkbox.

Upload a workflow to LiveDesign – Overwrite option application

To update an existing model

- QSAR model building
 - Local KNIME workflow
- QSAR prediction in LiveDesign

1. Prototyping

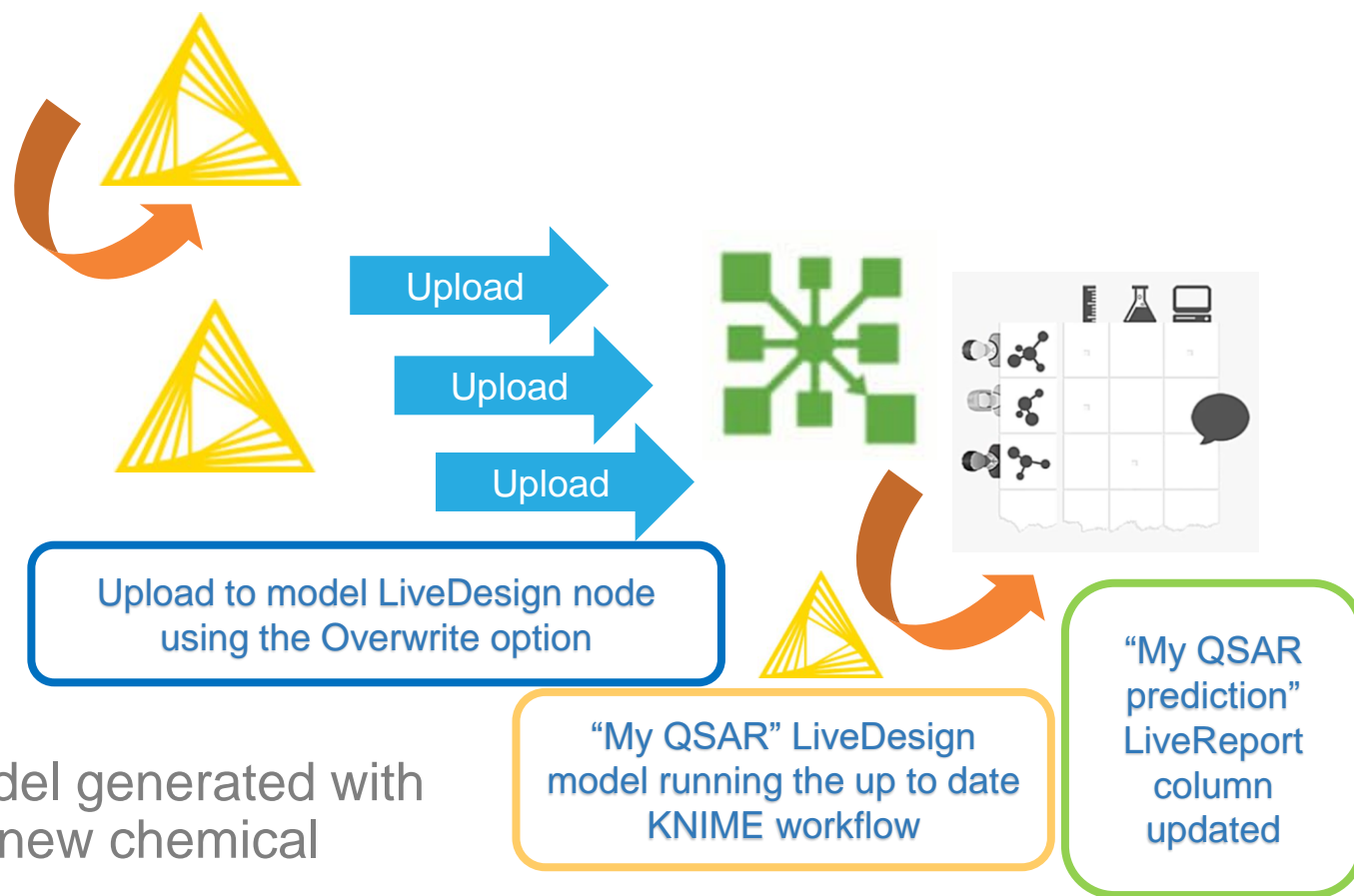
- Workflow fixes tested locally
- Then tested in LiveDesign

2. Improvements

- Uploaded and tested in LiveDesign

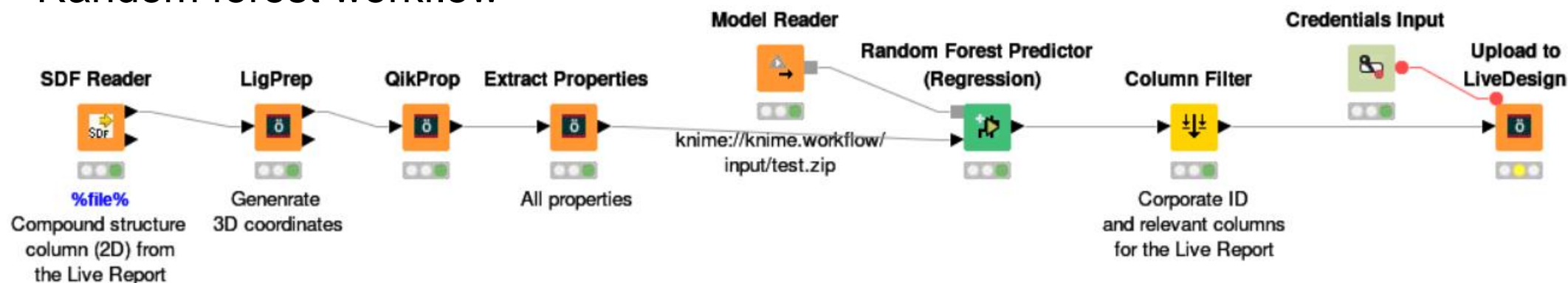
3. Updates

- With new versions of the QSAR model generated with the QSAR building workflow run on new chemical structures



Upload a workflow to LiveDesign – Application Example

- Random forest workflow



Summary:

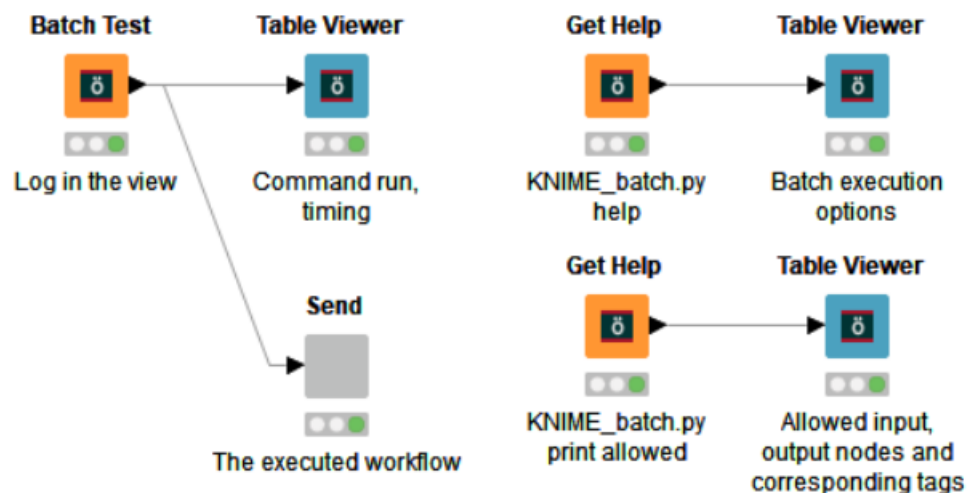
- The node makes it simple to add to LiveDesign any structure to text/numeric/structure workflow as model
- So the modelers can easily deploy their methods to LiveDesign to be used by the medicinal chemists

Minor Improvements and Fixes

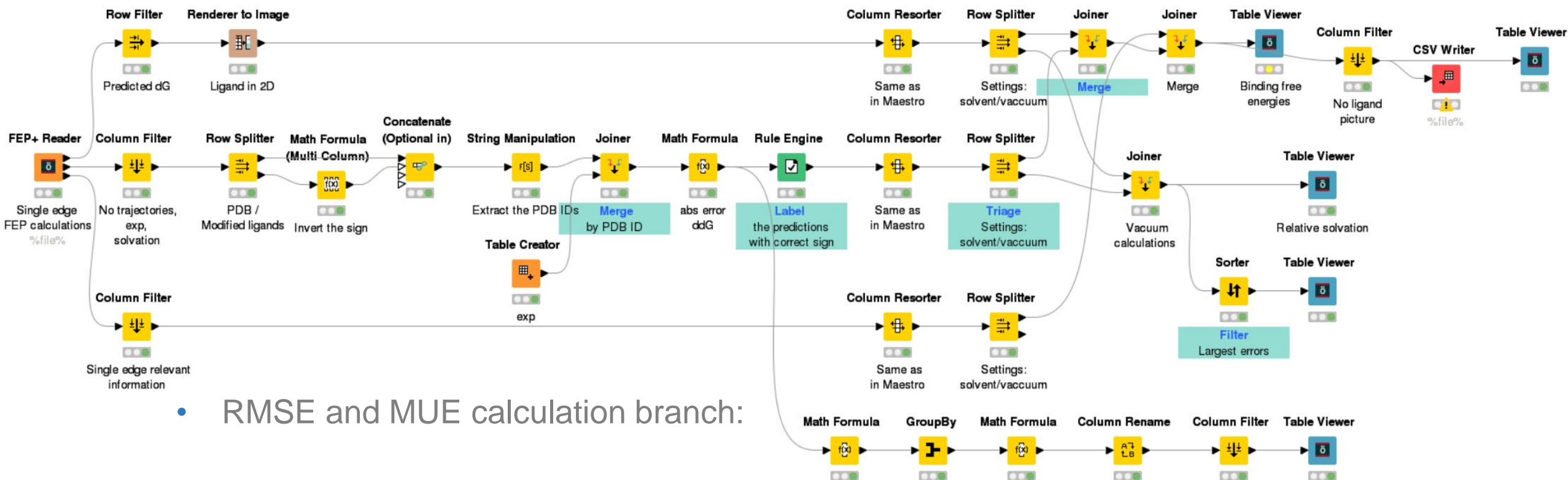
- The Schrodinger workflow examples are available on the KNIME hub:
 - https://hub.knime.com/schroedinger/spaces/Workflow_examples/latest
- The Schrodinger nodes can be install from the popup windows for missing nodes now they are available from the Partner update site.
- The Export to LiveDesign and Chemistry External Tool nodes are more robust
- The Blast node output the hit list ungrouped

New and Improved Workflow Examples

- LiveDesign – Upload model to LiveDesign
 - Epik and Docking workflows generating a new molecule column in the LiveReport
- Molecular Dynamics – Ligand alignment MD refinement
 - Improved version with the MD step and analysis step independant
- Tools – Batch execution
 - Using the new Batch test node. See the list of reader and writer nodes supported to be tagged.



Improved Workflow Example – FEP Analysis



- RMSE and MUE calculation branch:

| Row ID | S | S | Filename | D | FEP | D | experi... | D | abs er... | I | Correct sign | D | FEP Error | S | Energy Conv. | S | Lig. RMSD | S | REST Exch. | S | CCC Conv. | D | CCC | D | CCC Er... | D | Solvent Time | D | Compl... | S | Ligand1 | S | Ligand2 | S | PDB | S | Affinity... | S | Affinity | S | Type |
|--------------|-----|-----|---------------------------|-------|-------|---|-----------|---|-----------|------|--------------|-------|-----------|--------|--------------|-------------|--------------|------|------------|----------|-----------|---|-----|---|-----------|---|--------------|---|----------|---|---------|---|---------|---|-----|---|-------------|---|----------|---|------|
| Row3_Row2 | ... | ... | fep_F-H_1D3G_out.fmp | 2.17 | -0.92 | | | 0 | 0.014 | Good | Good | 2.17 | 0.01 | 4.999 | 4.999 | 1D3G_ligand | 1D3G_PDB | 1D3G | 8 | 1.7 | Ki | | | | | | | | | | | | | | | | | | | | |
| Row0_Row0 | ... | ... | fep_F-H_1BZH_out.fmp | -1.57 | 1.37 | | | 0 | 0.472 | Good | Bad | 0.472 | 0.47 | 29.999 | 29.999 | 1BZH_ligand | 1BZH_PDB | 1BZH | 1000 | 10000 | IC50 | | | | | | | | | | | | | | | | | | | | |
| Row0_Row1 | ... | ... | fep_F-H_1BZH_out.fmp | -1.57 | 1.37 | | | 0 | 0.472 | Good | Bad | 0.472 | 0.47 | 29.999 | 29.999 | 1BZH_ligand | 1BZH_PDB | 1BZH | 1000 | 10000 | IC50 | | | | | | | | | | | | | | | | | | | | |
| Row4_Row2 | ... | ... | fep_F-1d3g_mod_out.fmp | 2.02 | -0.92 | | | 0 | 0.022 | Good | Good | 2.02 | 0.02 | 4.999 | 4.999 | 1D3G_ligand | 1D3G_PDB | 1D3G | 8 | 1.7 | Ki | | | | | | | | | | | | | | | | | | | | |
| Row49_Row... | ... | ... | fep_F-H_3R17_out.fmp | 1.18 | -1.22 | | | 0 | 0.324 | Fair | Bad | 0.324 | 0.32 | 4.999 | 4.999 | 3R17_ligand | 3R17_PDB | 3R17 | 390 | 50 | Ki | | | | | | | | | | | | | | | | | | | | |
| Row26_Row... | ... | ... | fep_F-H_2IKI_out.fmp | 2.51 | 0.34 | | | 1 | 0.085 | Fair | Good | 0.085 | 0.09 | 4.999 | 4.999 | 2IKI_ligand | 2IKI_PDB | 2IKI | 4.00E+02 | 7.10E+02 | IC50 | | | | | | | | | | | | | | | | | | | | |
| Row55_Row... | ... | ... | fep_F-H_3UVP_out.fmp | -1.41 | 0.03 | | | 0 | 0.064 | Good | Fair | 0.064 | 0.06 | 4.999 | 4.999 | 3UVP_PDB | 3UVP_lig... | 3UVP | 35 | 37 | IC50 | | | | | | | | | | | | | | | | | | | | |
| Row51_Row... | ... | ... | fep_F-H_3SHY_out.fmp | 1.06 | -0.07 | | | 0 | 0.073 | Fair | Fair | 0.073 | 0.07 | 4.999 | 4.999 | 3SHY_ligand | 3SHY_PDB | 3SHY | 1700 | 1500 | Kd | | | | | | | | | | | | | | | | | | | | |
| Row53_Row... | ... | ... | fep_F-H_3TTZ_out.fmp | 2.02 | 0.95 | | | 1 | 0.057 | Good | Good | 0.057 | 0.06 | 4.999 | 4.999 | 3TTZ_PDB | 3TTZ_liga... | 3TTZ | 4 | 20 | IC50 | | | | | | | | | | | | | | | | | | | | |
| Row45_Row... | ... | ... | fep_F-H_3L1B_out.fmp | 1.12 | 0.08 | | | 1 | 0.022 | Good | Fair | 0.022 | 0.02 | 4.999 | 4.999 | 3L1B_PDB | 3L1B_liga... | 3L1B | 88 | 101 | EC50 | | | | | | | | | | | | | | | | | | | | |
| Row24_Row... | ... | ... | fep_F-H_2ATI_out.fmp | 1.6 | 0.61 | | | 1 | 0.064 | Fair | Fair | 0.064 | 0.06 | 4.999 | 4.999 | 2ATI_ligand | 2ATI_PDB | 2ATI | 22.91 | 64.57 | IC50 | | | | | | | | | | | | | | | | | | | | |
| Row18_Row... | ... | ... | fep_F-H_1YIN_out.fmp | 1.41 | 2.29 | | | 1 | 0.014 | Good | Good | 0.014 | 0.01 | 4.999 | 4.999 | 1YIN_ligand | 1YIN_PDB | 1YIN | 0.8 | 38 | IC50 | | | | | | | | | | | | | | | | | | | | |
| Row10_Row... | ... | ... | fep_F-H_1UK0_out.fmp | 0.79 | -0.08 | | | 0 | 0.067 | Fair | Good | 0.067 | 0.07 | 4.999 | 4.999 | 1UK0_PDB | 1UK0_liga... | 1UK0 | 16 | 14 | IC50 | | | | | | | | | | | | | | | | | | | | |
| Row20_Row... | ... | ... | fep_F-H_1YYE_out.fmp | -0.95 | -0.1 | | | 1 | 0.085 | Fair | Fair | 0.085 | 0.09 | 4.999 | 4.999 | 1YYE_ligand | 1YYE_PDB | 1YYE | 2.7 | 2.3 | IC50 | | | | | | | | | | | | | | | | | | | | |
| Row40_Row... | ... | ... | fep_F-H_3I81_out.fmp | 1.49 | 0.65 | | | 1 | 0.071 | Good | Good | 0.071 | 0.07 | 4.999 | 4.999 | 3I81_PDB | 3I81_ligand | 3I81 | 2 | 6 | IC50 | | | | | | | | | | | | | | | | | | | | |
| Row42_Row... | ... | ... | fep_F-H_3IOK_out.fmp | 0.41 | 1.15 | | | 1 | 0.064 | Good | Fair | 0.064 | 0.06 | 4.999 | 4.999 | 3IOK_ligand | 3IOK_PDB | 3IOK | 0.2 | 1.4 | IC50 | | | | | | | | | | | | | | | | | | | | |
| Row43_Row... | ... | ... | fep_F-H_3IOK_prot_out.fmp | 0.42 | 1.15 | | | 1 | 0.063 | Fair | Fair | 0.063 | 0.06 | 4.999 | 4.999 | 3IOK_ligand | 3IOK_PDB | 3IOK | 0.2 | 1.4 | IC50 | | | | | | | | | | | | | | | | | | | | |
| Row28_Row... | ... | ... | fep_F-H_2P3G_out.fmp | 0.23 | -0.38 | | | 0 | 0.063 | Good | Fair | 0.063 | 0.06 | 4.999 | 4.999 | 2P3G_PDB | 2P3G_lig... | 2P3G | 126 | 66 | IC50 | | | | | | | | | | | | | | | | | | | | |
| Row38_Row... | ... | ... | fep_F-H_3I6C_out.fmp | -0.08 | 0.5 | | | 0 | 0.196 | Fair | Bad | 0.196 | 0.2 | 4.999 | 4.999 | 3I6C_ligand | 3I6C_PDB | 3I6C | 12000 | 28000 | Ki | | | | | | | | | | | | | | | | | | | | |
| Row47_Row... | ... | ... | fep_F-H_3LBL_out.fmp | 0.32 | 0.87 | | | 1 | 0.045 | Good | Bad | 0.045 | 0.04 | 4.999 | 4.999 | 3LBL_ligand | 3LBL_PDB | 3LBL | 3 | 13 | Ki | | | | | | | | | | | | | | | | | | | | |
| Row57_Row... | ... | ... | fep_F-H_3ZC6_out.fmp | 0.4 | 0.93 | | | 1 | 0.022 | Good | Fair | 0.022 | 0.02 | 4.999 | 4.999 | 3ZC6_PDB | 3ZC6_lig... | 3ZC6 | 0.6 | 2.9 | IC50 | | | | | | | | | | | | | | | | | | | | |
| Row16_Row... | ... | ... | fep_F-H_1X7B_out.fmp | -0.71 | -0.21 | | | 1 | 0.102 | Fair | Fair | 0.102 | 0.1 | 4.999 | 4.999 | 1X7B_ligand | 1X7B_PDB | 1X7B | 5 | 3.5 | IC50 | | | | | | | | | | | | | | | | | | | | |

Analysis
Prediction summary:
RMSE, MUE



New features in the KNIME extension

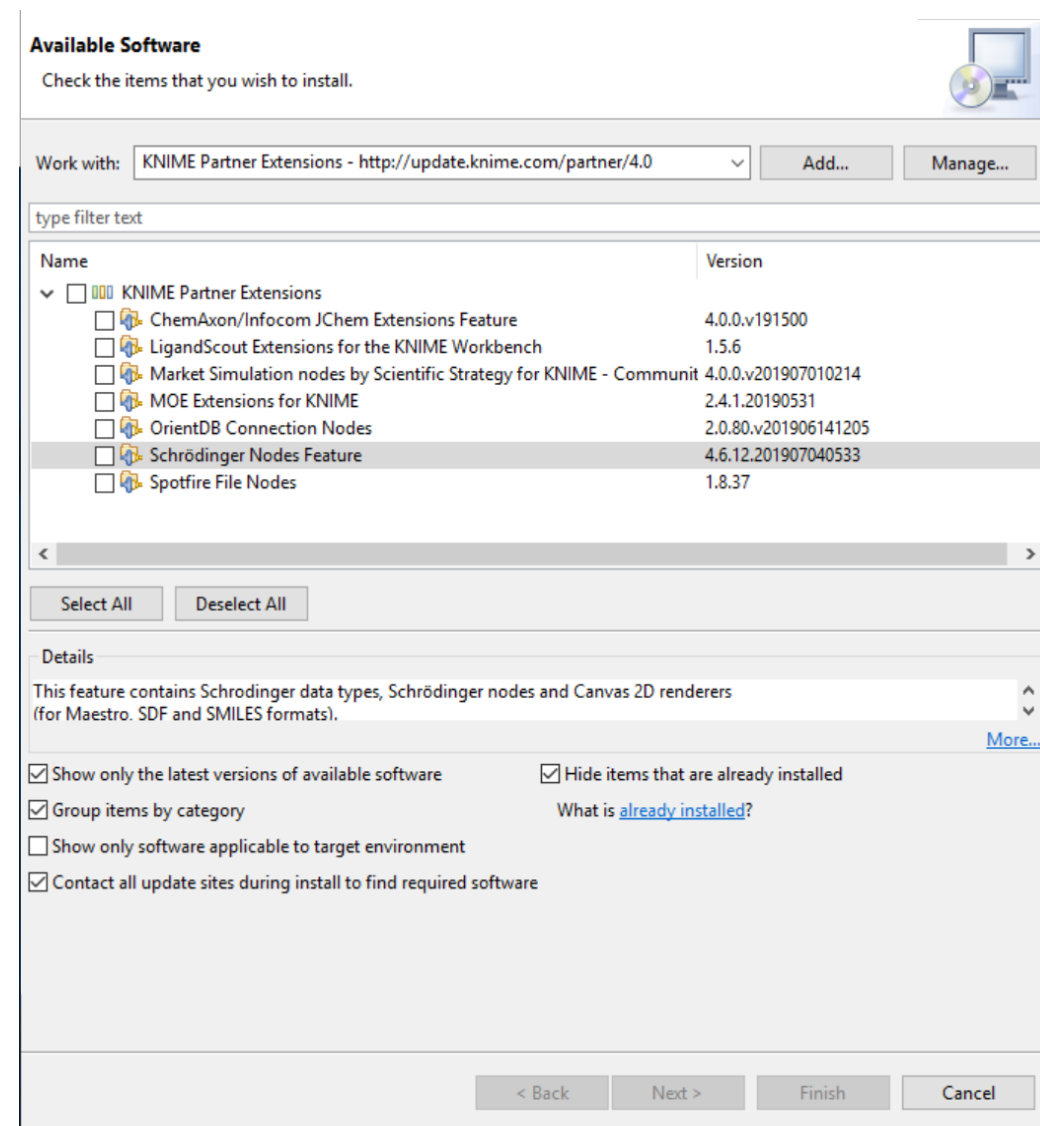
In Schrödinger Suite 2019-3

2019-3 New Features

- Supports the latest version of KNIME (v4.0)
- Our extensions are included in the new Partner update site
- New **FEP+ reader** node
- New node to easily **upload a workflow to LiveDesign** as model
- More reader and writer nodes are supported in KNIME_batch.py
- The Maestro reader and writer nodes can point to a directory inside the workflow

KNIME Analytics Platform 4.0

- Supports the latest version of KNIME (v4.0)
 - Not included yet because of a point to be fixed in KNIME 4.0.1. There is a workaround for now:
<https://www.schrodinger.com/node/411207>
The KNIME installation in the Schrodinger Suite can be updated easily (File > update KNIME) when the update is out.
 - Use the new Update site links that can be accessed without password:
<http://content.schrodinger.com/knime/extensions> and
<http://content.schrodinger.com/knime/previous>
- The new Partner update site includes our extensions
 - This is a central place to add commercial extensions
 - <http://update.knime.com/partner/4.0>



KNIME Analytics Platform 4.0 - some new features

See details on <https://www.knime.com/whats-new-in-knime-40> and KNIME Server 4.9

and the full list of changes:
<https://www.knime.com/changelog-v40>

KNIME Hub: for community workflows

KNIME Analytics Platform

- Components
- Performance
- Machine Learning, AWS ML Services Integration
- Duplicate Row Filter (per community request!)
 - select the columns identifying the duplicates. Supports various tie-breaking strategies and ways to just mark up the original table instead of outright filtering.
- Plotly Integration, Simplified Kerberos Support, KNIME Database Extension

Big Data : Spark Repartition, Revised Spark

Model Learner Nodes, Migration to the new KNIME Database Integration improvements

KNIME Server

- Remote Workflow Editor
- Scheduling Improvements
- Workflow Pinning (Distributed Executors)
 - Set up a heterogeneous set of executors
- Properties Editor
 - to control the behavior of workflows on KNIME Server (distribution)
- Create User Directories on First Login, Permissions for Individual Users

KNIME Server for AWS and Azure

General Release Note

- Community Extensions standardized the license schemes

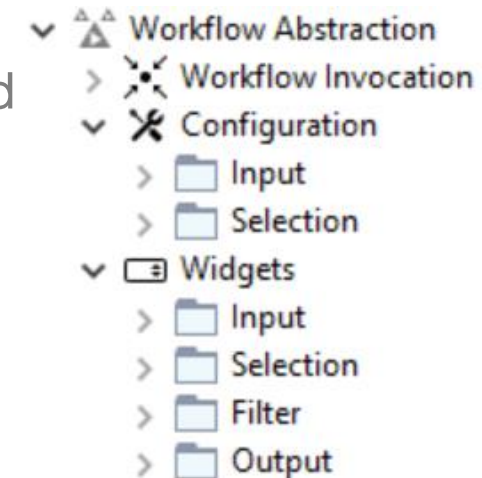
KNIME Analytics Platform 4.0 - some new features

- **Workflow hub**
 - <https://hub.knime.com> is the place for finding KNIME workflows, nodes, and components
 - Share workflows and components publicly with the entire KNIME community yourself. Use your KNIME account to log in to the newly added My-KNIME-Hub Mountpoint.
 - Browse KNIME extensions and learn about all nodes of an extension and explore related workflows to find examples on how to use this extension.
 - Drag and drop nodes or install extensions from the KNIME Hub into your running KNIME Analytics Platform workbench.
 - Search the KNIME Hub from within KNIME Analytics Platform
- **Python integration**
 - Simpler integration and issue debugging

KNIME Analytics Platform 4.0 - some new features

- Components

- Replace and enhance wrapped metanodes
- Encapsulate and abstract functionality. They are really nodes that you create with a workflow. They can have their own dialog and interactive views.
- Can be reused in your own workflows, shared with others via KNIME Server or the KNIME Hub, or represent web pages in an Analytical Application.
- The Quickform Nodes are deprecated and have been replaced with dedicated nodes for component configuration, input/output, and visualization widgets.
 - The old Quick form nodes still work in the new Components.



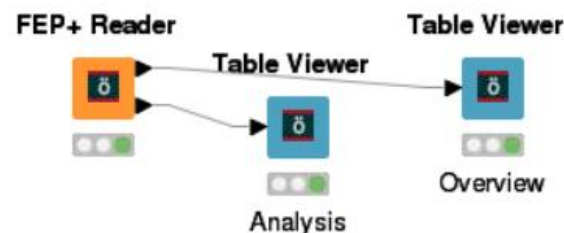
KNIME Server

- Remote Workflow Editor

- Edit workflows directly on KNIME Server.
- No need to download and upload a workflow when you make a small change
- Directly inspect a running workflow to view progress and debug
- Control a workflow that connects to secured resources
- Directly browse the KNIME Server repository from File Reader/Writer nodes

FEP+ reader node

- Reads -out.fmp files
 - Or all these files in a directory
- Same information as in Maestro FEP panel Overview and Analysis tabs
- Typical applications: merge, filter, triage and tag multiple single edge FEP runs
 - eg on the convergence criteria



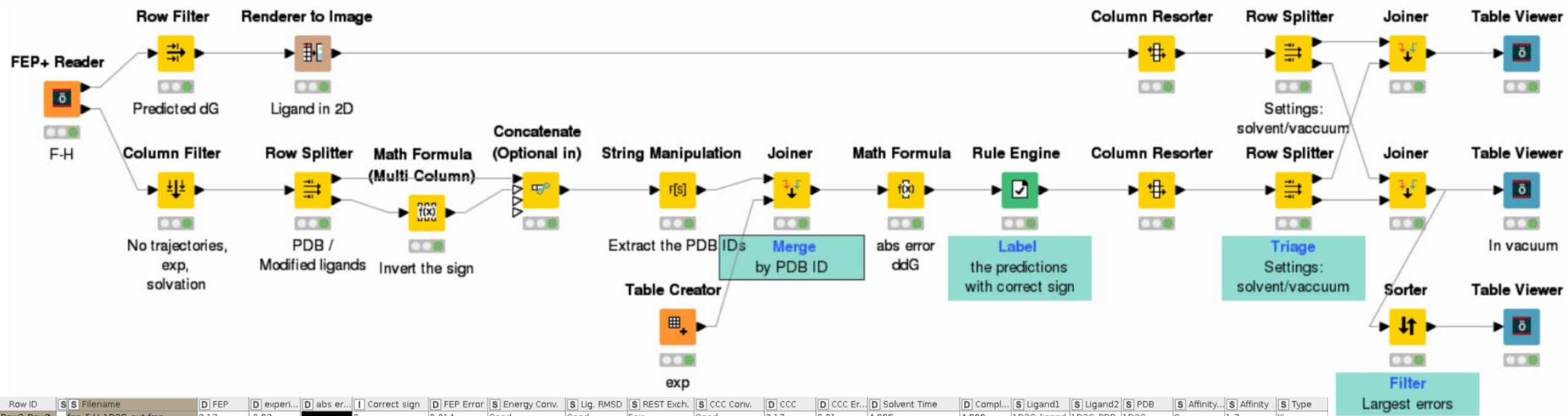
| Row ID | S Filename | S Ligand | D Pred. dG | D Pred Error | SM Structure |
|--------|----------------------|----------|------------|--------------|--------------|
| Row56 | fep_F-H_3UVP_out.fmp | 3UVP_PDB | 0 | 0.4 | |
| Row58 | fep_F-H_3ZC6_out.fmp | 3ZC6_PDB | 0 | 0.4 | |
| Row60 | fep_F-H_4AZ0_out.fmp | 4AZ0_PDB | 0 | 0.4 | |
| Row63 | fep_F-H_4B80_out.fmp | 4B80_PDB | -0.7 | 0.41 | |
| Row65 | fep_F-H_4B82_out.fmp | 4B82_PDB | 0.38 | 0.41 | |
| Row67 | fep_F-H_4BCD_out.fmp | 4BCD_PDB | -0.35 | 0.41 | |
| Row68 | fep_F-H_4CSJ_out.fmp | 4CSJ_PDB | 0 | 0.4 | |
| Row70 | fep_F-H_4EJN_out.fmp | 4EJN_PDB | 0 | 0.4 | |

File Hilite Navigation View

Table "default" - Rows: 46 Spec - Columns: 20 Properties Flow Variables

| Row ID | S Filename | S Ligand1 | S Ligand2 | D Exp. | D FEP | D FEP Error | D CCC | D CCC Error | D Solvation | D Solvation Error | S Energy Conv. | S Lig. RMSD | S REST Exch. | S CCC Conv. | D Solvent Time | D Complex... | S Solvent Trajectory 1 | S Solvent Trajectory 2 | S Complex Trajectory 1 | S Complex Trajectory 2 |
|--------|----------------------|-------------|--------------|--------|-------|-------------|-------|-------------|-------------|-------------------|----------------|-------------|--------------|-------------|----------------|--------------|-------------------------------|-------------------------------|-------------------------------|-------------------------------|
| Row0 | fep_F-H_1BZH_out.fmp | 1BZH_ligand | 1BZH_PDB | ? | 1.57 | 0.472 | 1.57 | 0.47 | ? | ? | Good | Bad | Fair | Good | 29.999 | 29.999 | Trajectory Location:"/tmp/... | Trajectory Location:"/tmp/... | Trajectory Location:"/tmp/... | Trajectory Location:"/tmp/... |
| Row1 | fep_F-H_1BZH_vacu... | 1D3G_ligand | 1D3G_PDB | ? | -2.17 | 0.014 | -2.17 | 0.01 | ? | ? | Good | Good | Fair | Good | 4.999 | 4.999 | Trajectory Location:"/tmp/... | Trajectory Location:"/tmp/... | Trajectory Location:"/tmp/... | Trajectory Location:"/tmp/... |
| Row2 | fep_F-H_1D3G_out.fmp | 1D3G_ligand | 1D3G_PDB | ? | -2.17 | 0.014 | -2.17 | 0.01 | ? | ? | Good | Good | Fair | Good | 4.999 | 4.999 | Trajectory Location:"/tmp/... | Trajectory Location:"/tmp/... | Trajectory Location:"/tmp/... | Trajectory Location:"/tmp/... |
| Row3 | fep_F-H_1GSZ_out.fmp | 1GSZ_PDB | 1GSZ_lig... | ? | 0.64 | 0.085 | 0.64 | 0.09 | ? | ? | Fair | Fair | Fair | Good | 4.999 | 4.999 | Trajectory Location:"/tmp/... | Trajectory Location:"/tmp/... | Trajectory Location:"/tmp/... | Trajectory Location:"/tmp/... |
| Row4 | fep_F-H_1Q1M_out.fmp | 1Q1M_ligand | 1Q1M_PDB | ? | -0.1 | 0.273 | -0.1 | 0.27 | ? | ? | Fair | Good | Fair | Good | 4.999 | 4.999 | Trajectory Location:"/tmp/... | Trajectory Location:"/tmp/... | Trajectory Location:"/tmp/... | Trajectory Location:"/tmp/... |
| Row5 | fep_F-H_1UK0_out.fmp | 1UK0_PDB | 1UK0_liga... | ? | 0.79 | 0.067 | 0.79 | 0.07 | ? | ? | Fair | Good | Fair | Good | 4.999 | 4.999 | Trajectory Location:"/tmp/... | Trajectory Location:"/tmp/... | Trajectory Location:"/tmp/... | Trajectory Location:"/tmp/... |
| Row6 | fep_F-H_1UK1_out.fmp | 1UK1_PDB | 1UK1_liga... | ? | 0.79 | 0.022 | 0.79 | 0.02 | ? | ? | Good | Good | Fair | Good | 4.999 | 4.999 | Trajectory Location:"/tmp/... | Trajectory Location:"/tmp/... | Trajectory Location:"/tmp/... | Trajectory Location:"/tmp/... |
| Row7 | fep_F-H_1W6J_out.fmp | 1W6J_ligand | 1W6J_PDB | ? | -0.2 | 0.143 | -0.2 | 0.14 | ? | ? | Fair | Good | Fair | Good | 4.999 | 4.999 | Trajectory Location:"/tmp/... | Trajectory Location:"/tmp/... | Trajectory Location:"/tmp/... | Trajectory Location:"/tmp/... |
| Row8 | fep_F-H_1X7B_out.fmp | 1X7B_ligand | 1X7B_PDB | ? | 0.71 | 0.102 | 0.71 | 0.1 | ? | ? | Fair | Fair | Fair | Good | 4.999 | 4.999 | Trajectory Location:"/tmp/... | Trajectory Location:"/tmp/... | Trajectory Location:"/tmp/... | Trajectory Location:"/tmp/... |
| Row9 | fep_F-H_1YIN_out.fmp | 1YIN_ligand | 1YIN_PDB | ? | -1.41 | 0.014 | -1.41 | 0.01 | ? | ? | Good | Good | Fair | Good | 4.999 | 4.999 | Trajectory Location:"/tmp/... | Trajectory Location:"/tmp/... | Trajectory Location:"/tmp/... | Trajectory Location:"/tmp/... |
| Row10 | fep_F-H_1YYE_out.fmp | 1YYE_ligand | 1YYE_PDB | ? | 0.95 | 0.085 | 0.95 | 0.09 | ? | ? | Fair | Fair | Fair | Good | 4.999 | 4.999 | Trajectory Location:"/tmp/... | Trajectory Location:"/tmp/... | Trajectory Location:"/tmp/... | Trajectory Location:"/tmp/... |
| Row11 | fep_F-H_1Z73_out.fmp | 1Z73_PDB | 1Z73_lig... | ? | 0.69 | 0.093 | 0.69 | 0.09 | ? | ? | Fair | Fair | Fair | Good | 4.999 | 4.999 | Trajectory Location:"/tmp/... | Trajectory Location:"/tmp/... | Trajectory Location:"/tmp/... | Trajectory Location:"/tmp/... |

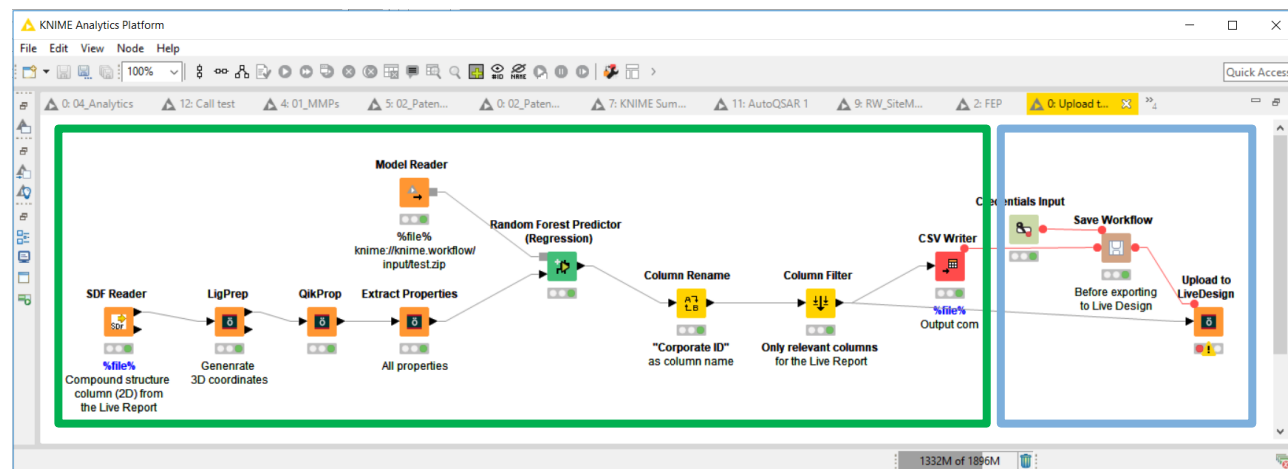
FEP reader node – application



| Row ID | S | S | Filename | D | FEP | D | experi... | D | abs er... | I | Correct sign | D | FEP Error | S | Energy Conv. | S | Lig. RMSD | S | REST Exch. | S | CCC Conv. | D | CCC | D | CCC Er... | D | Solvent Time | D | Compl... | S | Ligand1 | S | Ligand2 | S | PDB | S | Affinity... | S | Affinity | S | Type |
|--------------|-----|-----|---------------------------|-------|-------|---|-----------|------|-----------|------|--------------|-------|-----------|--------|--------------|-------------|--------------|------|------------|----------|-----------|---|-----|---|-----------|---|--------------|---|----------|---|---------|---|---------|---|-----|---|-------------|---|----------|---|------|
| Row3_Row2 | ... | ... | fep_F-H_1D3G_out.fmp | 2.17 | -0.92 | 0 | 0.014 | Good | Good | Fair | Good | 2.17 | 0.01 | 4.999 | 4.999 | 1D3G_ligand | 1D3G_PDB | 1D3G | 8 | 1.7 | Ki | | | | | | | | | | | | | | | | | | | | |
| Row0_Row0 | ... | ... | fep_F-H_1BZH_out.fmp | -1.57 | 1.37 | 0 | 0.472 | Good | Bad | Fair | Good | -1.57 | 0.47 | 29.999 | 29.999 | 1BZH_ligand | 1BZH_PDB | 1BZH | 1000 | 10000 | IC50 | | | | | | | | | | | | | | | | | | | | |
| Row0_Row1 | ... | ... | fep_F-H_1BZH_out.fmp | -1.57 | 1.37 | 0 | 0.472 | Good | Bad | Fair | Good | -1.57 | 0.47 | 29.999 | 29.999 | 1BZH_ligand | 1BZH_PDB | 1BZH | 1000 | 10000 | IC50 | | | | | | | | | | | | | | | | | | | | |
| Row4_Row2 | ... | ... | fep_F-H_1d3g_mod_out.fmp | 2.02 | -0.92 | 0 | 0.022 | Good | Good | Fair | Good | 2.02 | 0.02 | 4.999 | 4.999 | 1D3G_ligand | 1D3G_PDB | 1D3G | 8 | 1.7 | Ki | | | | | | | | | | | | | | | | | | | | |
| Row49_Row... | ... | ... | fep_F-H_3R17_out.fmp | 1.18 | -1.22 | 0 | 0.324 | Fair | Bad | Fair | Good | 1.18 | 0.32 | 4.999 | 4.999 | 3R17_ligand | 3R17_PDB | 3R17 | 390 | 50 | Ki | | | | | | | | | | | | | | | | | | | | |
| Row26_Row... | ... | ... | fep_F-H_2IKI_out.fmp | 2.51 | 0.34 | 1 | 0.085 | Fair | Good | Fair | Good | 2.51 | 0.09 | 4.999 | 4.999 | 2IKI_ligand | 2IKI_PDB | 2IKI | 4.00E+02 | 7.10E+02 | IC50 | | | | | | | | | | | | | | | | | | | | |
| Row55_Row... | ... | ... | fep_F-H_3UVP_out.fmp | -1.41 | 0.03 | 0 | 0.064 | Good | Fair | Fair | Good | -1.41 | 0.06 | 4.999 | 4.999 | 3UVP_PDB | 3UVP_lig... | 3UVP | 35 | 37 | IC50 | | | | | | | | | | | | | | | | | | | | |
| Row51_Row... | ... | ... | fep_F-H_3SHY_out.fmp | 1.06 | -0.07 | 0 | 0.073 | Fair | Fair | Fair | Good | 1.06 | 0.07 | 4.999 | 4.999 | 3SHY_ligand | 3SHY_PDB | 3SHY | 1700 | 1500 | Kd | | | | | | | | | | | | | | | | | | | | |
| Row53_Row... | ... | ... | fep_F-H_3TTZ_out.fmp | 2.02 | 0.95 | 1 | 0.057 | Good | Good | Fair | Good | 2.02 | 0.06 | 4.999 | 4.999 | 3TTZ_PDB | 3TTZ_liga... | 3TTZ | 4 | 20 | IC50 | | | | | | | | | | | | | | | | | | | | |
| Row45_Row... | ... | ... | fep_F-H_3L1B_out.fmp | 1.12 | 0.08 | 1 | 0.022 | Good | Fair | Fair | Good | 1.12 | 0.02 | 4.999 | 4.999 | 3L1B_PDB | 3L1B_liga... | 3L1B | 88 | 101 | EC50 | | | | | | | | | | | | | | | | | | | | |
| Row24_Row... | ... | ... | fep_F-H_2ATI_out.fmp | 1.6 | 0.61 | 1 | 0.064 | Fair | Fair | Fair | Good | 1.6 | 0.06 | 4.999 | 4.999 | 2ATI_ligand | 2ATI_PDB | 2ATI | 22.91 | 64.57 | IC50 | | | | | | | | | | | | | | | | | | | | |
| Row18_Row... | ... | ... | fep_F-H_1YIN_out.fmp | 1.41 | 2.29 | 1 | 0.014 | Good | Good | Fair | Good | 1.41 | 0.01 | 4.999 | 4.999 | 1YIN_ligand | 1YIN_PDB | 1YIN | 0.8 | 38 | IC50 | | | | | | | | | | | | | | | | | | | | |
| Row10_Row... | ... | ... | fep_F-H_1UK0_out.fmp | 0.79 | -0.08 | 0 | 0.067 | Fair | Good | Fair | Good | 0.79 | 0.07 | 4.999 | 4.999 | 1UK0_PDB | 1UK0_liga... | 1UK0 | 16 | 14 | IC50 | | | | | | | | | | | | | | | | | | | | |
| Row20_Row... | ... | ... | fep_F-H_1YYE_out.fmp | -0.95 | -0.1 | 1 | 0.085 | Fair | Fair | Fair | Good | -0.95 | 0.09 | 4.999 | 4.999 | 1YYE_ligand | 1YYE_PDB | 1YYE | 2.7 | 2.3 | IC50 | | | | | | | | | | | | | | | | | | | | |
| Row40_Row... | ... | ... | fep_F-H_3I81_out.fmp | 1.49 | 0.65 | 1 | 0.071 | Good | Good | Fair | Good | 1.49 | 0.07 | 4.999 | 4.999 | 3I81_PDB | 3I81_ligand | 3I81 | 2 | 6 | IC50 | | | | | | | | | | | | | | | | | | | | |
| Row42_Row... | ... | ... | fep_F-H_3I0K_out.fmp | 0.41 | 1.15 | 1 | 0.064 | Good | Fair | Fair | Good | 0.41 | 0.06 | 4.999 | 4.999 | 3I0K_ligand | 3I0K_PDB | 3I0K | 0.2 | 1.4 | IC50 | | | | | | | | | | | | | | | | | | | | |
| Row43_Row... | ... | ... | fep_F-H_3I0K_prot_out.fmp | 0.42 | 1.15 | 1 | 0.063 | Fair | Fair | Fair | Good | 0.42 | 0.06 | 4.999 | 4.999 | 3I0K_ligand | 3I0K_PDB | 3I0K | 0.2 | 1.4 | IC50 | | | | | | | | | | | | | | | | | | | | |
| Row28_Row... | ... | ... | fep_F-H_2P3G_out.fmp | 0.23 | -0.38 | 0 | 0.063 | Good | Fair | Fair | Good | 0.23 | 0.06 | 4.999 | 4.999 | 2P3G_PDB | 2P3G_lig... | 2P3G | 126 | 66 | IC50 | | | | | | | | | | | | | | | | | | | | |
| Row38_Row... | ... | ... | fep_F-H_3I6C_out.fmp | -0.08 | 0.5 | 0 | 0.196 | Fair | Bad | Fair | Good | -0.08 | 0.2 | 4.999 | 4.999 | 3I6C_ligand | 3I6C_PDB | 3I6C | 12000 | 28000 | Ki | | | | | | | | | | | | | | | | | | | | |
| Row47_Row... | ... | ... | fep_F-H_3LBL_out.fmp | 0.32 | 0.87 | 1 | 0.045 | Good | Bad | Fair | Good | 0.32 | 0.04 | 4.999 | 4.999 | 3LBL_ligand | 3LBL_PDB | 3LBL | 3 | 13 | Ki | | | | | | | | | | | | | | | | | | | | |
| Row57_Row... | ... | ... | fep_F-H_3ZC6_out.fmp | 0.4 | 0.93 | 1 | 0.022 | Good | Fair | Fair | Good | 0.4 | 0.02 | 4.999 | 4.999 | 3ZC6_PDB | 3ZC6_lig... | 3ZC6 | 0.6 | 2.9 | IC50 | | | | | | | | | | | | | | | | | | | | |
| Row16_Row... | ... | ... | fep_F-H_1X7B_out.fmp | -0.71 | -0.21 | 1 | 0.102 | Fair | Fair | Fair | Good | -0.71 | 0.1 | 4.999 | 4.999 | 1X7B_ligand | 1X7B_PDB | 1X7B | 5 | 3.5 | IC50 | | | | | | | | | | | | | | | | | | | | |
| Row32_Row... | ... | ... | fep_F-H_2YDJ_out.fmp | -0.04 | 0.41 | 0 | 0.042 | Good | Good | Fair | Good | -0.04 | 0.04 | 4.999 | 4.999 | 2YDJ_ligand | 2YDJ_PDB | 2YDJ | 5 | 10 | IC50 | | | | | | | | | | | | | | | | | | | | |
| Row30_Row... | ... | ... | fep_F-H_2VTD_out.fmp | 0.55 | 0.13 | 1 | 0.058 | Good | Fair | Fair | Good | 0.55 | 0.06 | 4.999 | 4.999 | 2VTD_ligand | 2VTD_PDB | 2VTD | 8.50E+04 | 105000 | IC50 | | | | | | | | | | | | | | | | | | | | |
| Row22_Row... | ... | ... | fep_F-H_1Z22_out.fmp | 0.98 | 0.58 | 1 | 0.081 | Fair | Fair | Fair | Good | 0.98 | 0.08 | 4.999 | 4.999 | 1Z22_PDB | 1Z22_lig... | 1Z22 | 6000 | 16000 | IC50 | | | | | | | | | | | | | | | | | | | | |
| Row12_Row... | ... | ... | fep_F-H_1UK1_out.fmp | 0.79 | 0.41 | 1 | 0.022 | Good | Good | Fair | Good | 0.79 | 0.02 | 4.999 | 4.999 | 1UK1_PDB | 1UK1_liga... | 1UK1 | 60 | 120 | IC50 | | | | | | | | | | | | | | | | | | | | |
| Row6_Row3 | ... | ... | fep_F-H_1GSZ_out.fmp | 0.64 | 0.28 | 1 | 0.085 | Fair | Fair | Fair | Good | 0.64 | 0.09 | 4.999 | 4.999 | 1GSZ_PDB | 1GSZ_lig... | 1GSZ | 60 | 96 | IC50 | | | | | | | | | | | | | | | | | | | | |
| Row14_Row... | ... | ... | fep_F-H_1W6J_out.fmp | 0.2 | -0.11 | 0 | 0.143 | Fair | Good | Fair | Good | 0.2 | 0.14 | 4.999 | 4.999 | 1W6J_ligand | 1W6J_PDB | 1W6J | 6.5 | 5.4 | IC50 | | | | | | | | | | | | | | | | | | | | |
| Row36_Row... | ... | ... | fep_F-H_3EY4_out.fmp | 0.87 | 0.62 | 1 | 0.054 | Fair | Fair | Fair | Good | 0.87 | 0.05 | 4.999 | 4.999 | 3EY4_ligand | 3EY4_PDB | 3EY4 | 35 | 100 | Ki | | | | | | | | | | | | | | | | | | | | |

Upload a workflow to LiveDesign – Workflow

- In my workflow in KNIME
 - Label the SDF input and CSV output nodes
 - Execute the Upload model to LiveDesign node
 - The workflow is uploaded to LiveDesign as Model using a generic KNIME Protocol



- In the LiveReport

- Add the column(s)

The KNIME workflow is run behind the scene

Global

DATA & COLUMNS

Open Live Report + Global 05/21/19

Project Favorites

Computed Properties

Computational Models

KNIME

 Upload to Live Design

 Upload to Live Design - Random forest

 Add All

 Prediction (QPlogBB)

 Prediction (QPlogBB) (Prediction Variance)

 QPlogBB

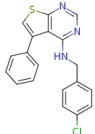
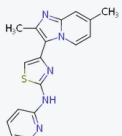
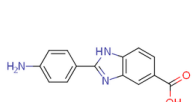
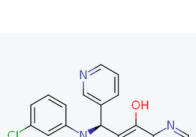
Experimental Assays

Other Columns

Formulas

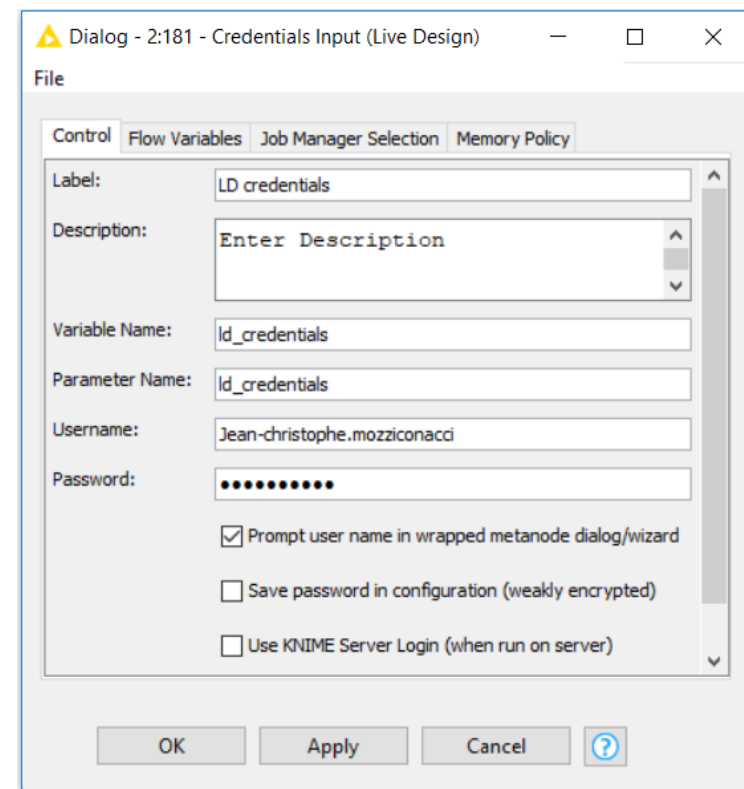
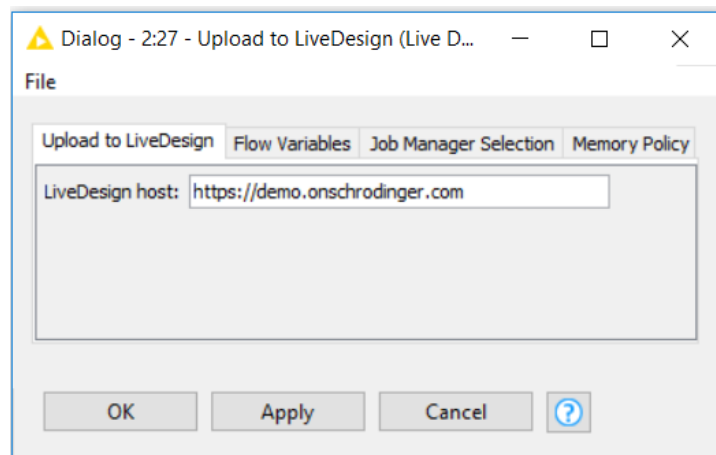
Multi-Parameter Profiles

Freeform Columns

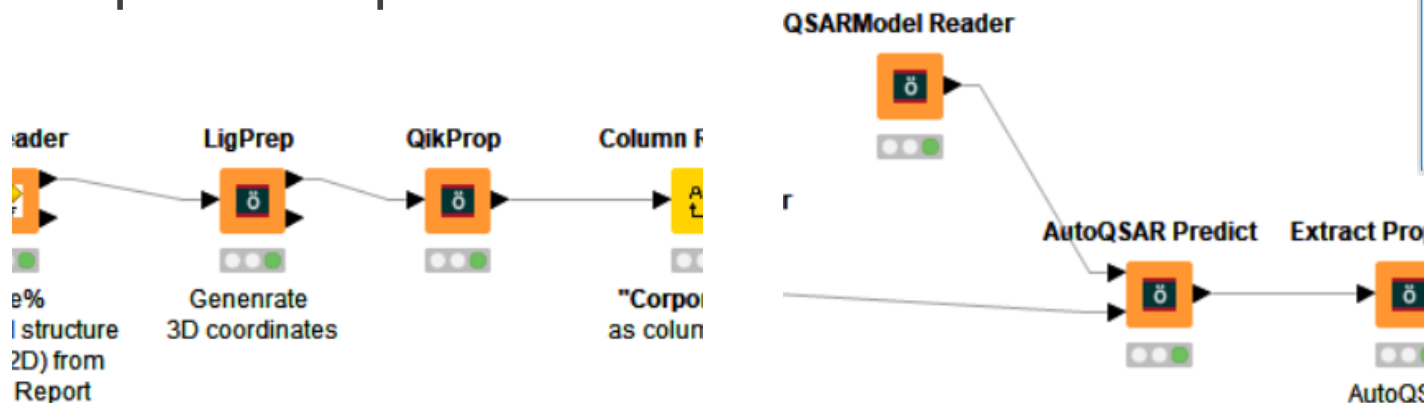
| | Compound Structure | ID | All IDs | 3D (3D) | Upload to Live Design (Extensions) | Upload to Live Design (Test) |
|---|---|--------|---------|---------|------------------------------------|------------------------------|
| 1 |  | V35000 | V35000 | | | |
| 2 |  | V35002 | V35002 | | | |
| 3 |  | V35006 | V35006 | | | |
| 4 |  | V35010 | V35010 | | | |

Upload a workflow to LiveDesign

- Any workflow with a structure input and text/numeric output can be uploaded as LiveDesign model



- Simple examples



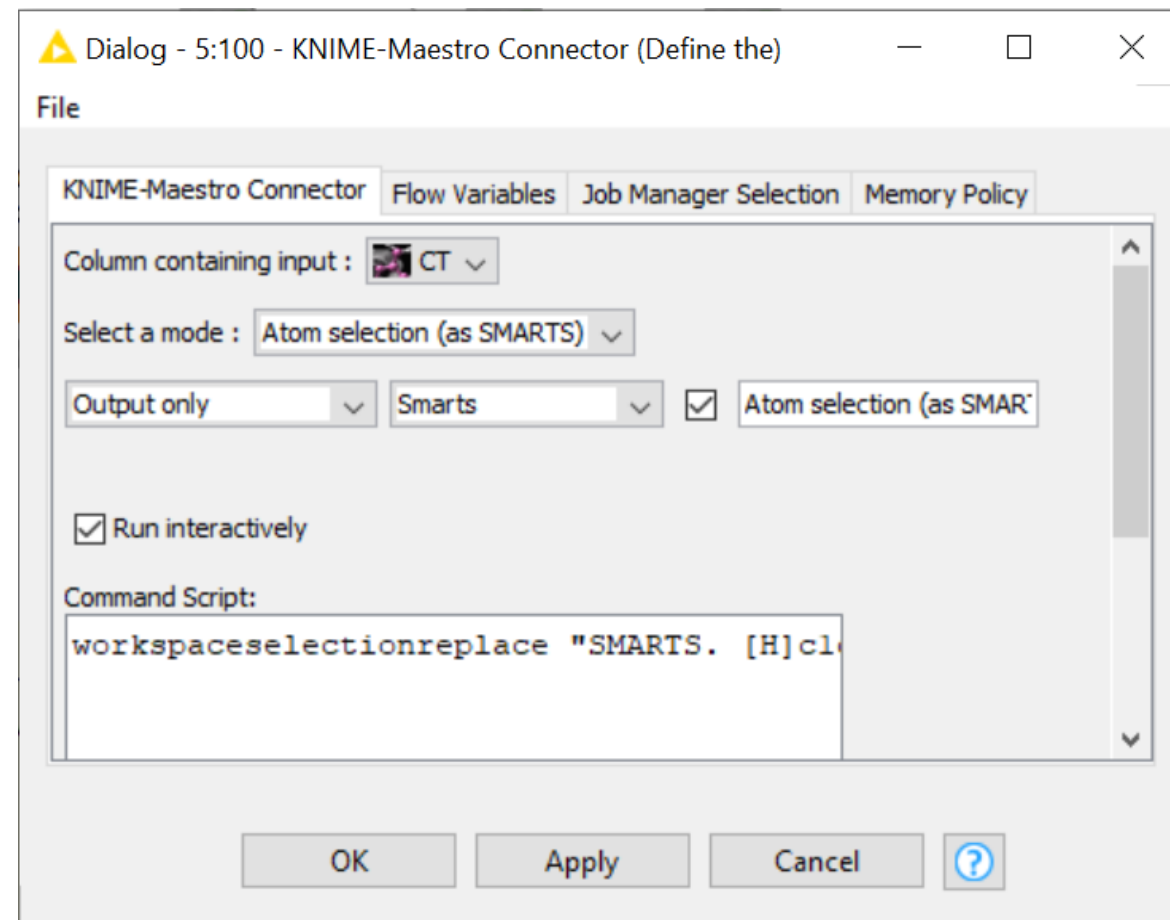
Reader and writer node improvements

- More reader and writer nodes are supported by KNIME_batch.py
 - KNIME Model reader, CMS file reader, AutoQSAR model reader and writer nodes
 - So these nodes can be controlled in LiveDesign models
- The Maestro reader and writer nodes can point to a directory inside the workflow
 - Using `knime://knime.workflow/<path>/<filename>`
 - Application: store input structures for Reader nodes
 - No reconfiguration is required for someone to test the workflow on the same inputs
 - The workflow can be reset and rerun while keeping the required QSAR models, query or reference structures...

For instance when run in LiveDesign or on the KNIME Server

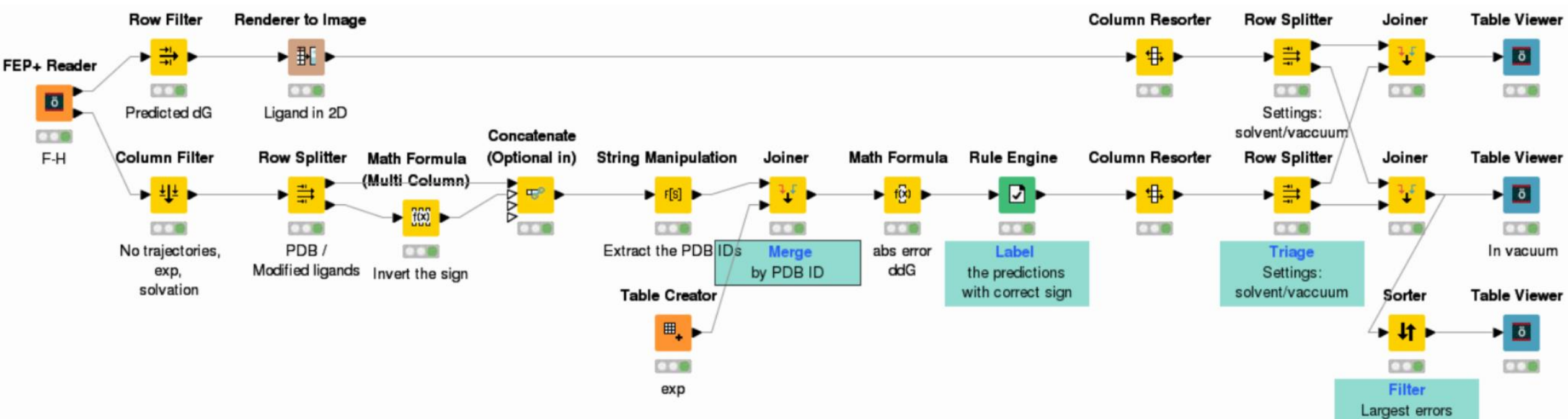
Minor Improvements and Fixes

- Run interactively toggle button in the KNIME-Maestro connector node
 - Easily switch between the interactive and the automatic modes
 - You can test a workflow opening Maestro for interactive manipulations. Then switch mode before sending it to a colleague. So it runs automatically and doesn't require manual intervention.
- The Automatic Compound Extraction node is more robust



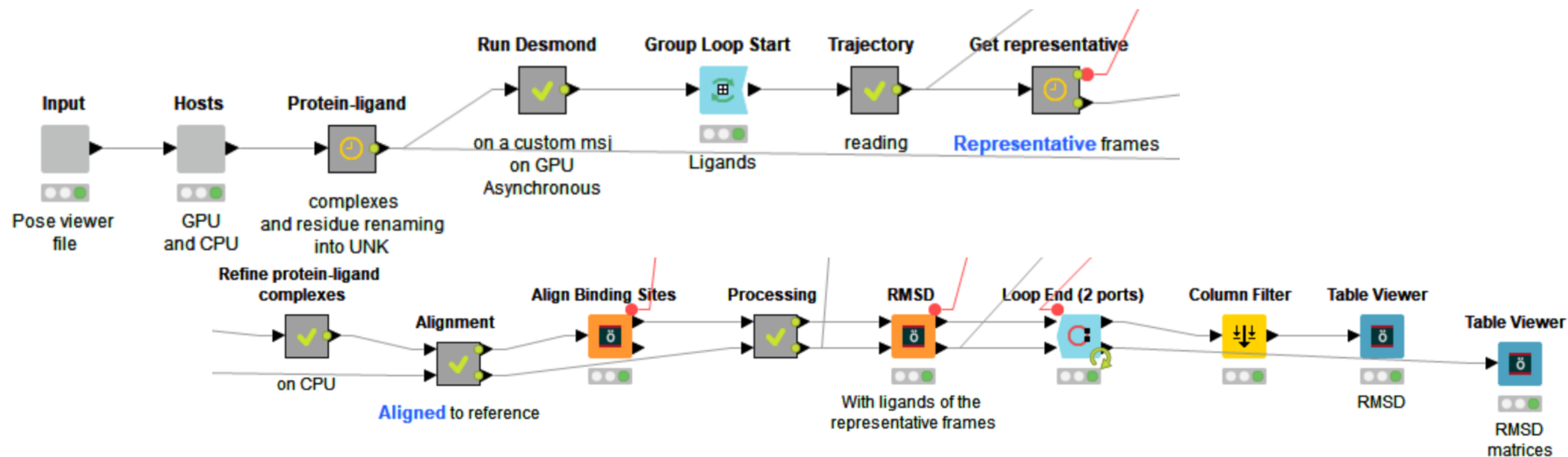
New and Improved Workflow Examples

- **Molecular Dynamics – FEP analysis**
 - An overview (predictions along with the ligand 2D structures) of a set of single edge FEP calculations is given as well as analysis details (including errors and conversion checking). So results can be labelled, triaged, filtered, and extra data can be merged.



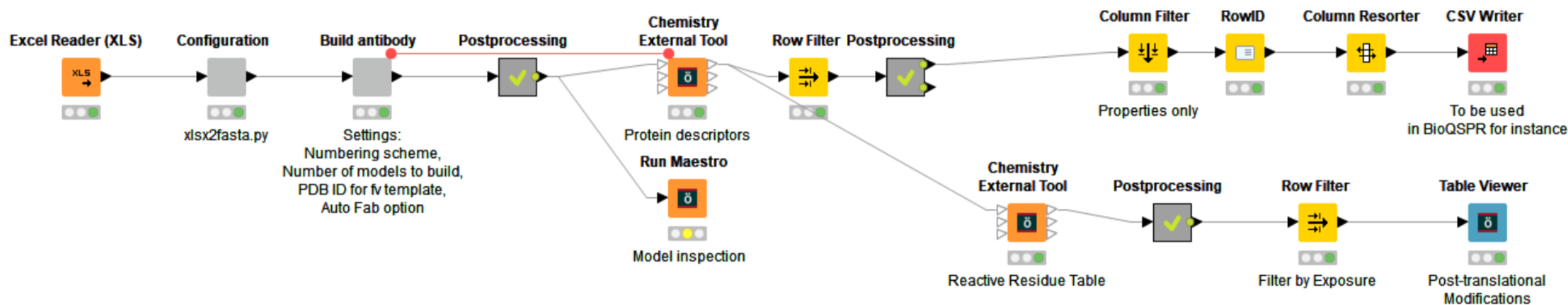
New and Improved Workflow Examples

- Molecular Dynamics – Ligand alignment MD refinement
 - A Desmond molecular dynamics simulation is run on each ligand prealigned in the protein binding site. Then the representative frames are refined with Prime and the RMSDs are reported to assess the pose stability.
 - The workflow can be used to refine for instance on a docking based alignment to prepare the input of a FEP calculation.



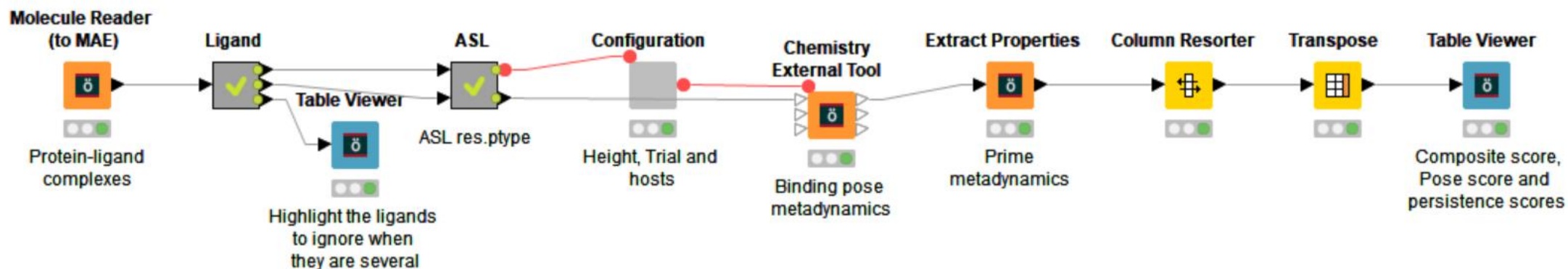
New and Improved Workflow Examples

- LiveDesign – Upload model to LiveDesign
 - QikProp, Docking, Random forest workflow examples
- Protein – Build antibody models
 - Improvements: Sequences can be read from an XLS spreadsheet. Post-translational modifications and protein descriptors are calculated for each model and the latter can be used as input to BioQSPR.



New and Improved Workflow Examples

- Molecular Dynamics – Metadynamics
 - To rank binding site conformations of a ligand in a single binding site



- Protein – missing loop refinement
 - Refine all the loops added using 'Fill loops' option in the Protein Preparation node



New features in the KNIME extension

In Schrödinger Suite 2019-2

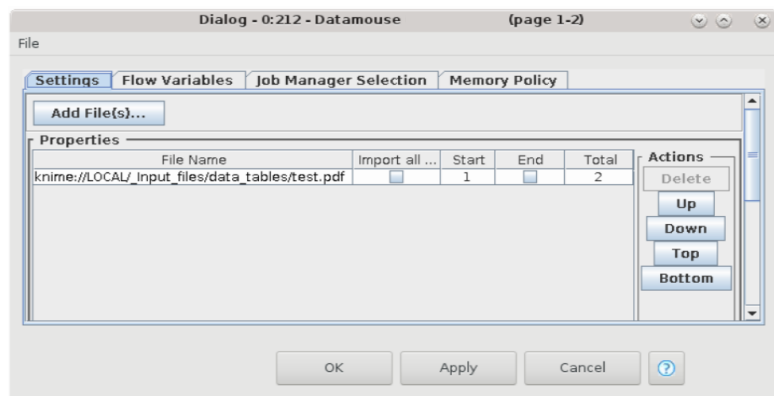
2019-2 New Features

- Includes the latest version of KNIME on all platforms
- New Automatic Compound Extraction node
- Glide ligand docking node settings can be imported from a Maestro calculation
- The Desmond trajectory nodes handle FEP trajectories

[KNIME Schrödinger extensions version 4.6]

Automatic Compound Extraction node

- Extract the structures from a pdf document from the whole document or specified page



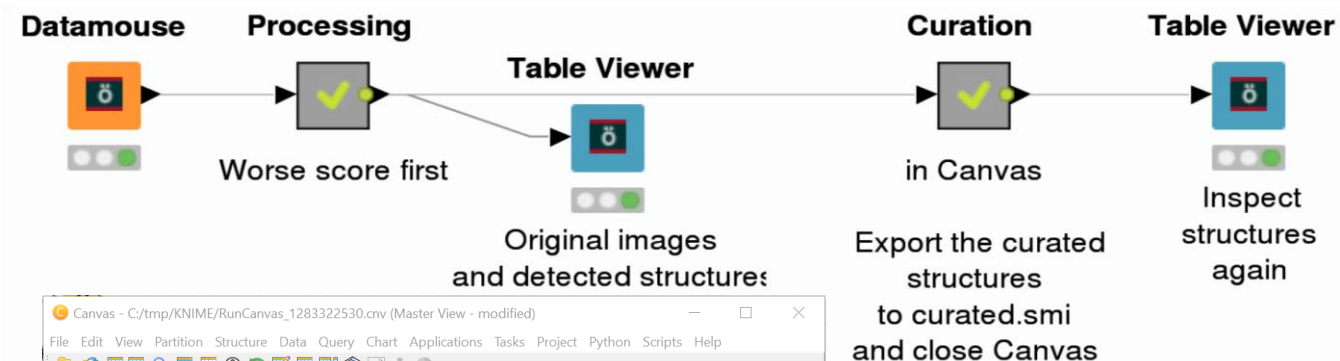
- The output smiles column can be compared with corresponding document section images

| Row ID | Page | rendered_predictions | SM predicted_smiles_SplitResultList | D scores_... |
|---------|------|----------------------|-------------------------------------|--------------|
| Row3_17 | 3 | | | 98.053 |
| Row1_1 | 1 | | | 98.065 |
| Row6_3 | 6 | | | 98.074 |
| Row5_23 | 5 | | | 98.215 |

Automatic Compound Extraction - Structure curation in Canvas

- Select the structures to fix
- Manually curated in Canvas
 - Started from the node
 - Double click on the structure to edit
 - Irrelevant structures can be deleted before exportation
- or in Maestro

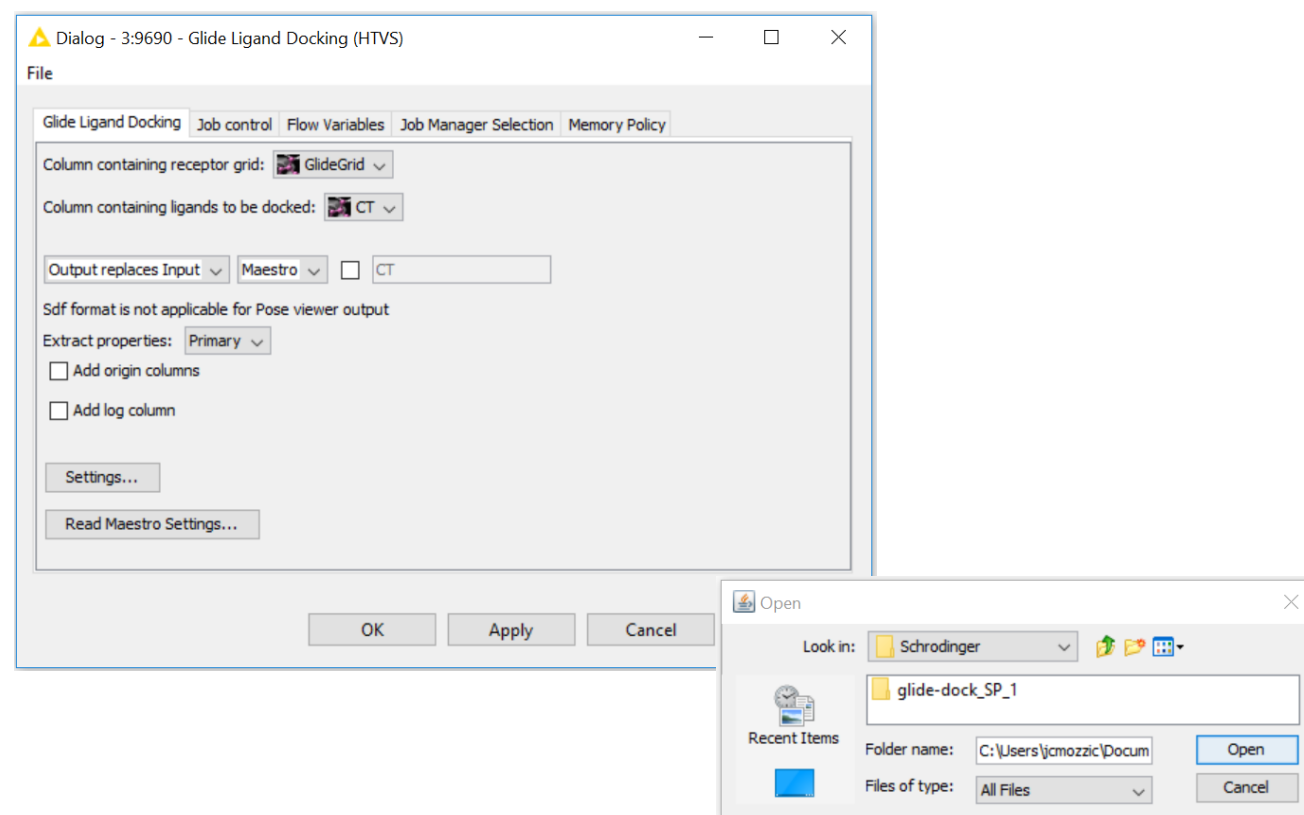
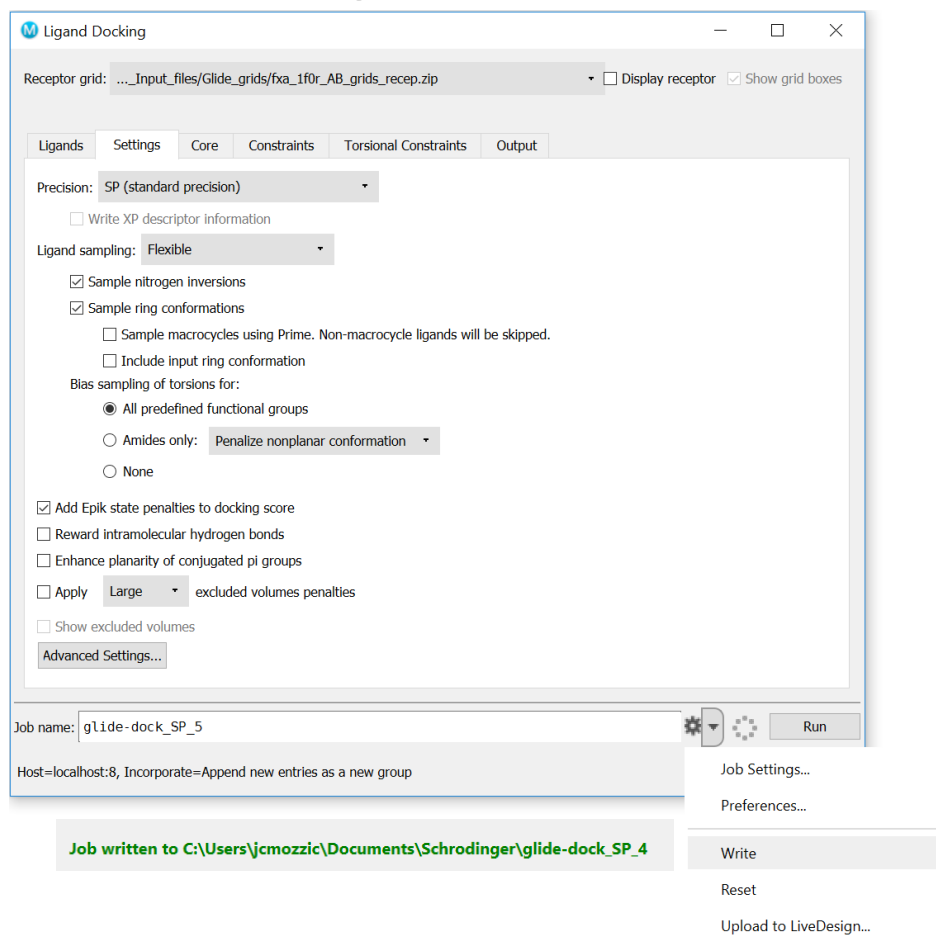
| Row ID | Page | rendered_predictions | aa predicted_smiles_SplitResultList | D scores... |
|---------|------|----------------------|-------------------------------------|-------------|
| Row6_16 | 6 | | | 99.756 |
| Row2_9 | 2 | | | 99.818 |
| Row5_11 | 5 | | | 99.859 |
| Row6_12 | 6 | | | 99.89 |



The screenshot shows the Canvas application window with a table of chemical structures. The table has columns for Row ID, Structure, and D scores. The structure in Row 5_11 is highlighted. An 'Edit Structure' dialog box is open, showing the chemical structure of the selected row. The dialog box has buttons for OK, Cancel, and Help.

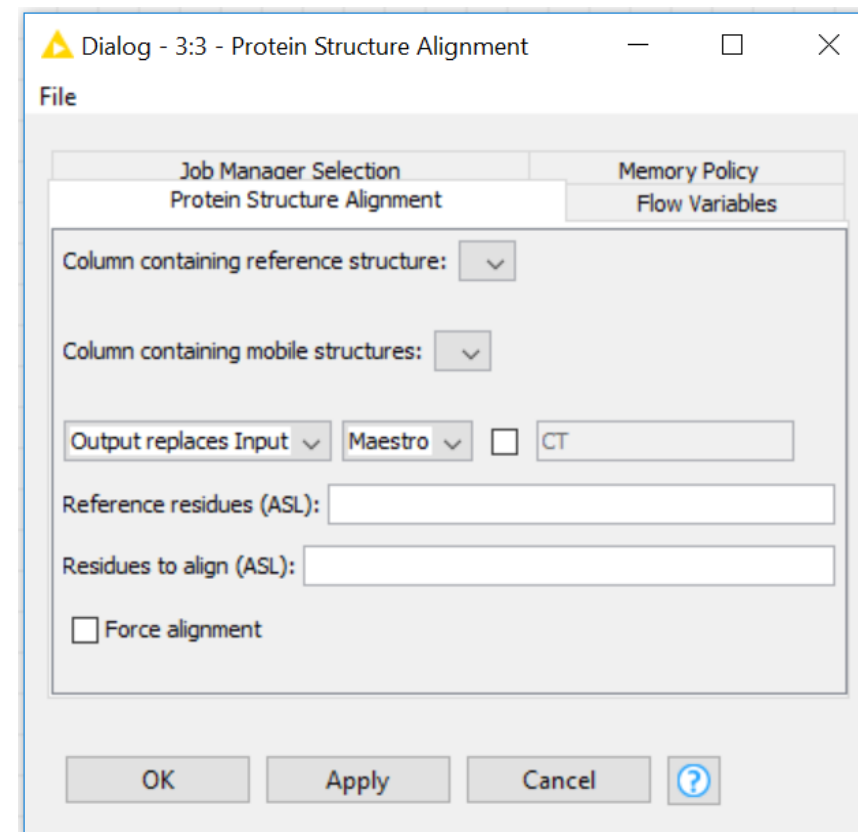
Glide ligand docking node settings from a Maestro calculation

- Once the Glide settings have been tested in Maestro, use the Write button
- The setting file can be read from the node to set up the configuration panel



Other improvements

- Includes the latest version of KNIME (v3.7)
 - The Mac version has also been updated
- Desmond trajectory nodes handle FEP trajectories
 - Snapshots stored in fmp files
- The Protein Structure Alignment node configuration panel includes all the ASL options available in Maestro

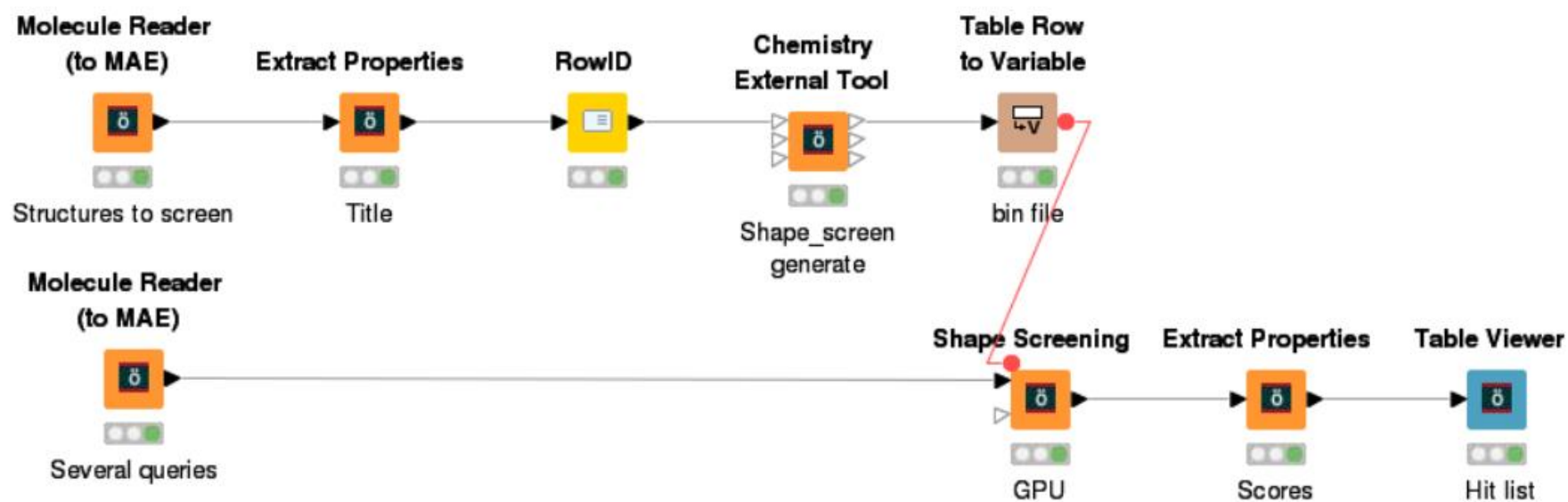


New and Improved Workflow Examples

- Quantum Mechanics – Conformer and tautomer prediction
 - Generate and rank possible tautomers
- Quantum Mechanics – QM descriptors
 - Runs qm_descriptors.py to start a series of jobs and harvest molecular (including Dipole Moment, HOMO/LUMO, isodensity surface contributions, Internal energy, energy components, enthalpy, entropy and Gibbs free energy contributions) and atomic descriptors (including charges, Fukui indices, electrostatic potential, NMR shielding, spin densities).
- General – Automatic Compound Extraction
 - Structure extraction and curation
- Server – AutoQSAR
 - Runs the AutoQSAR node on a KNIME Server to predict a molecule sketched in the Webportal

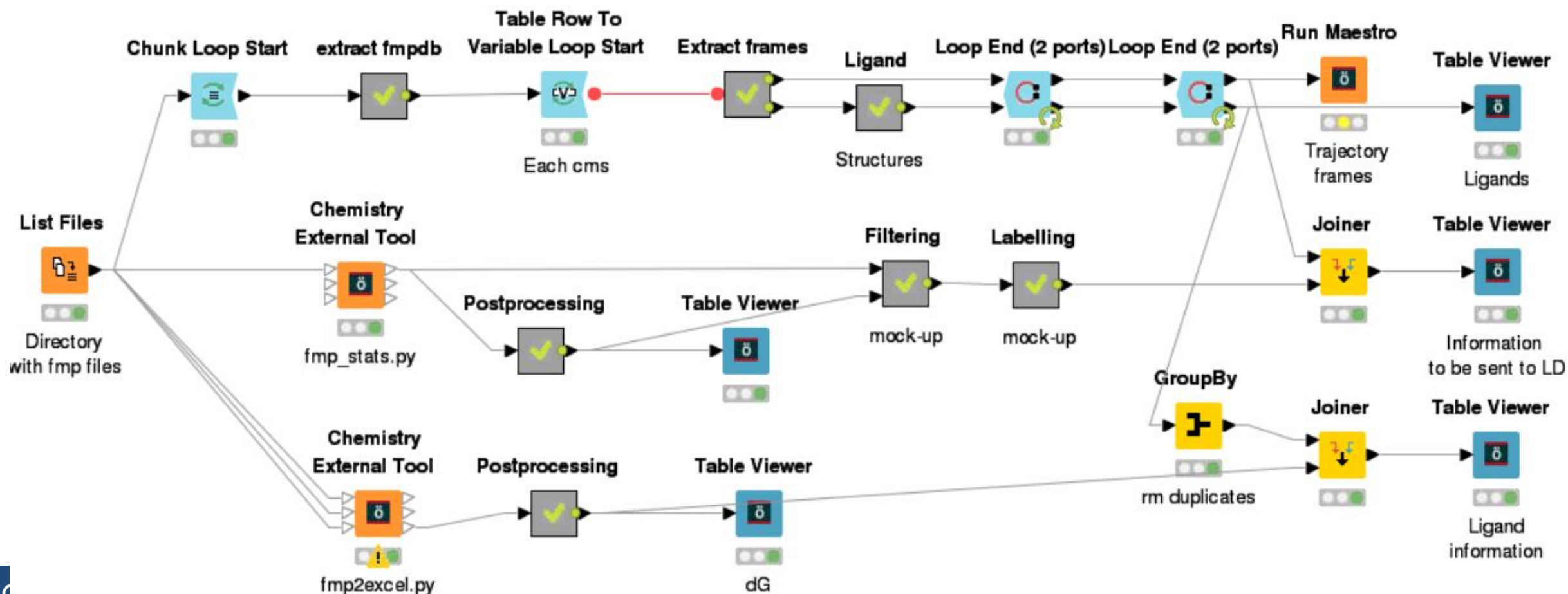
New and Improved Workflow Examples

- Pharmacophore – Shape screening
 - Creates the bin file and runs the Shape screening on GPU



New and Improved Workflow Examples

- Molecular Dynamics – FEP trajectory information
 - It extracts the trajectory snapshots, ligand 2D structures and some fmp data available through command line scripts (including the predictions, bad edges, edge connectivity).





New features in the KNIME extension

In Schrödinger Suite 2019-1

2019-1 New Features

- Includes the latest version of KNIME (v3.7.0)
- New Conformer and tautomer prediction node
- New Semiempirical NDDO node
- The Shape screening node runs on GPUs
- New AutoQSAR model writer node

[KNIME Schrödinger extensions version 4.5]

KNIME Analytics Platform 3.7 - some new features

See details on <https://www.knime.com/whats-new-in-knime-37> and KNIME Server 4.8

and the full list of changes in the <https://www.knime.com/changelog-v37>

KNIME Analytics Platform

- New Statistics Nodes
- Jupyter Integration
 - your code can stay in Jupyter but still be used from within your KNIME workflows
- XGBoost machine learning library Integration
 - Linear Ensemble or Tree Ensemble learners
- Google Authentication and Google Drive Connectivity
- Updated Tableau Integration
- Usability Improvements - Zooming with the Keyboard (CTRL + and CTRL -)

Guided Analytics and New Views

- Heatmap
- Hierarchical Cluster Assigner
- Tile View
- CSS Editor
 - Fine control over the styling of the JavaScript views in your KNIME WebPortal applications (or in Composite Views in KNIME Analytics Platform).

Interactive Layout Editor and Nested Wrapped Metanodes

- WebPortal page or wrapped metanode composite view: you can now use a drag and drop interface to layout your page.
- Wrapped metanodes can be included inside other wrapped metanodes. This allows you to build up a library of wrapped metanodes that contain useful linked views and then easily assemble them to create complex views for visualizing and interacting with datasets.

Big Data

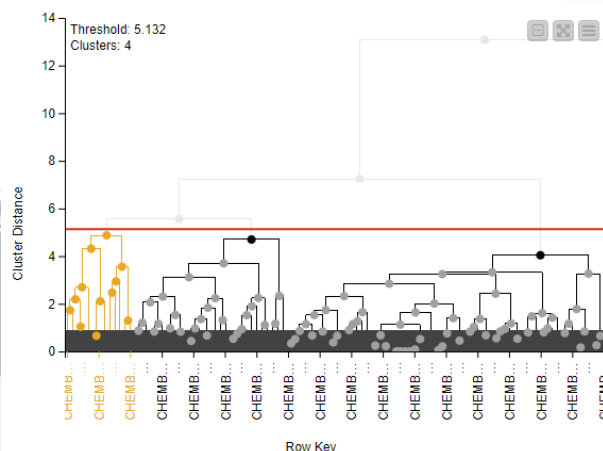
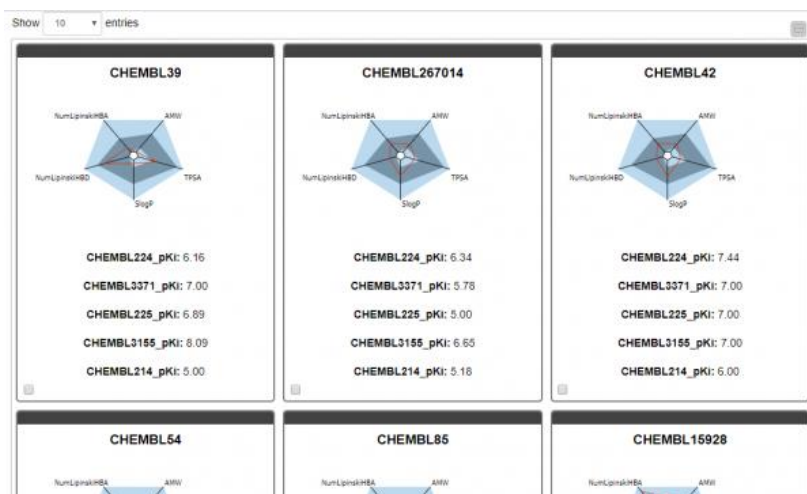
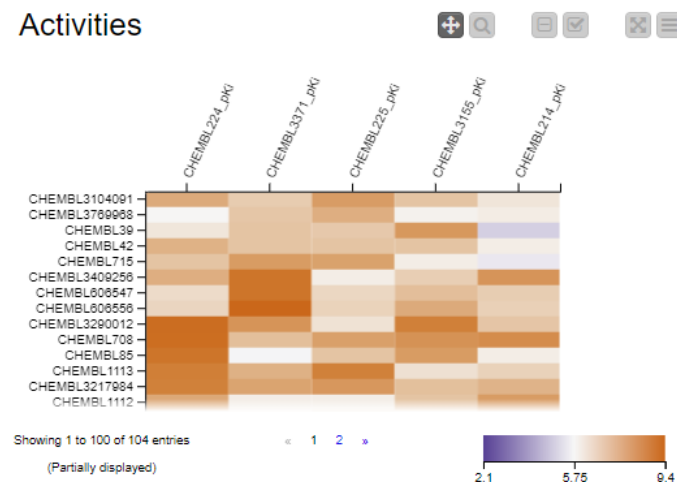
- PySpark Node Collection, Spark Row Filter, Apache Livy Support, Support for Spark 2.4

KNIME Server

- Distributed Executors
 - KNIME Server to scale workflow execution by adding (or removing) executors that can each run one or more workflows.
- Remote Workflow Editor (Preview)
 - The Remote Workflow Editor allows KNIME Analytics Platform users to view, edit, and execute workflows on KNIME Server. Take advantage of powerful server hardware, get direct access to protected resources like databases, and monitor the progress of key workflows as they're executing.
- Management Services for KNIME Analytics Platform: Customization
- Performance Enhancements
 - Copy multiple files from your Analytics Platform to KNIME Server.
- Monitor Job Execution Time
- New Database Framework (Preview)

KNIME Analytics Platform 3.7 - some new features

Activities



New Workflow Annotation

- Arrange
- Connect selected nodes
- Disconnect selected nodes
- Collapse into Metanode

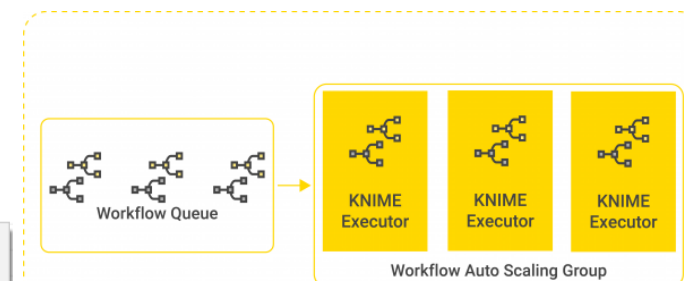
Bring Annotation to Front (Ctrl+Shift+PageUp)
Bring Annotation Forward (Ctrl+PageUp)
Send Annotation Backward (Ctrl+PageDown)
Send Annotation to Back (Ctrl+Shift+PageDown)

Dialog - 2:243 - Python Script (1=1)

```
nb = knime_jupyter.load_notebook(notebook_directory="knime://knime.workflow/../jupyter_notebooks",  
                                notebook_name="tsNE_for_text.ipynb", only_include_tag='export')  
vectors = list(input_table['topic_vect'])  
coords = nb.run_tsNE_for_vectors(vectors, random_state=0x#00d)  
output_table = input_table.copy()  
output_table['X'] = coords[:,0]  
output_table['Y'] = coords[:,1]
```

jupyter tsNE_for_text Last Checkpoint: 11/09/2018 (autosaved)

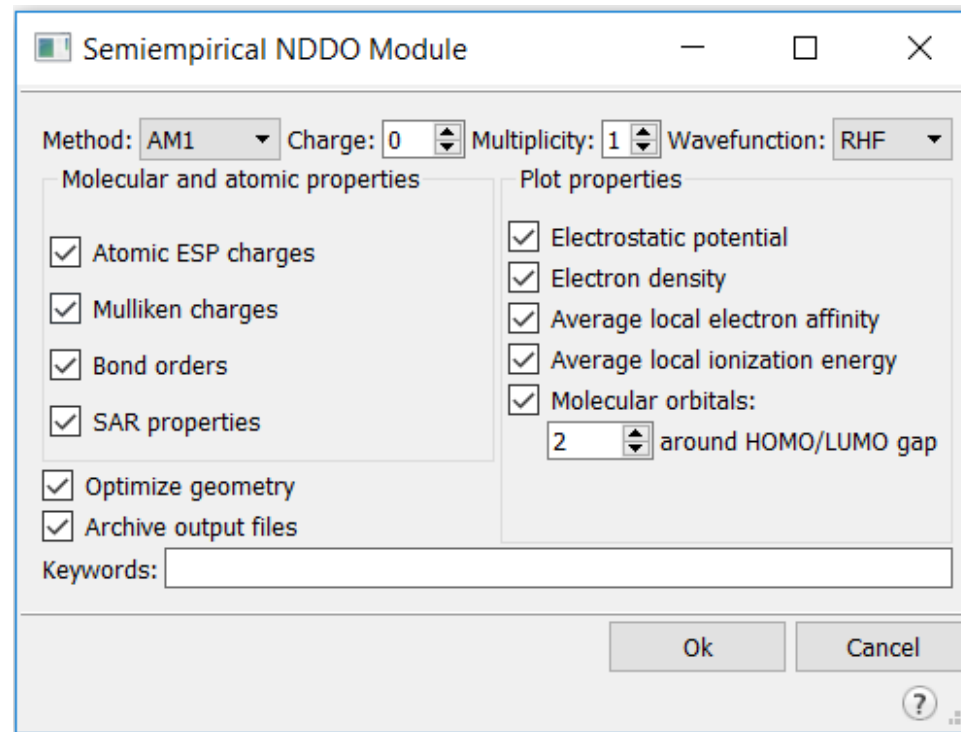
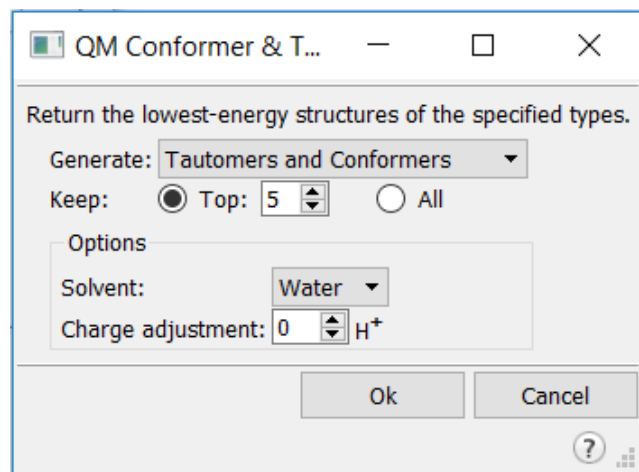
```
from sklearn import manifold  
from sklearn.metrics import pairwise  
import numpy as np  
from rdkit import DataStructs  
def run_tsNE_for_vectors(vectors, **kwargs):  
    dists = pairwise.euclidean_distances(vectors)  
    mdl = manifold.TSNE(metric='precomputed', **kwargs)  
    pts_embedded = mdl.fit_transform(dists)  
    return pts_embedded
```



KNIME Server Distributed Executors

Conformer and tautomer prediction and Semiempirical NDDO nodes

- New nodes using the same configuration panel as Maestro





New features in the KNIME extension

In Schrödinger Suite 2018-4

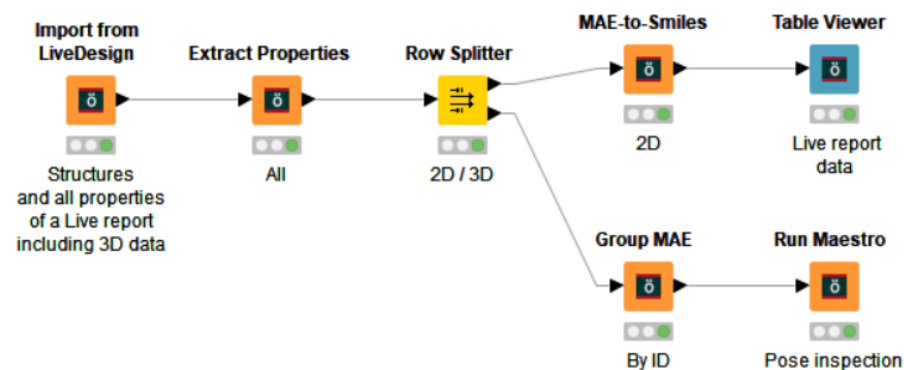
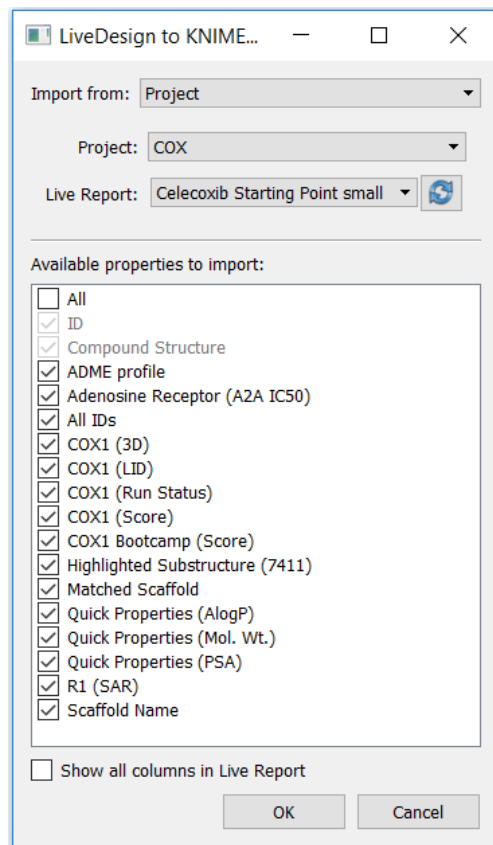
2018-4 New Features

- The **Import from LiveDesign** node can import 3D data
- Job files can be viewed with the **Jobcontrol node**
- New **Postmortem node**
- The Run Canvas node takes sdf and smiles columns as input

[KNIME Schrödinger extensions version 4.4]

LiveDesign Import Node

- 3D structures can be imported



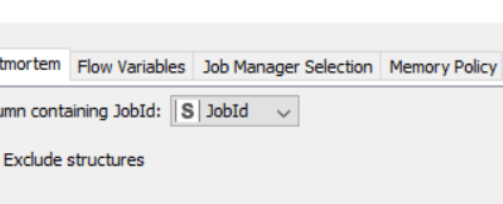
Job control node and Postmortem new node

- Job files can be viewed with the Jobcontrol node

So as to inspect the calculation status while it's running

- Postmortem new node

| Row ID | S File Path | Txt File Contents |
|--------|---|--|
| Row0 | C:\Users\jcmozic\AppData\Local\Temp\prepwizard_1728391405_1.log | <p>Working on structure 1</p> <p>Fixing common structure mistakes...</p> <p>No mistakes were found</p> <p>Assigning bond orders...</p> <p>Using CCD: True</p> <p>CCD template assignment successfully used for</p> <p>CCD template assignment successfully used for</p> <p>CCD template assignment successfully used for</p> <p>Assigned the following bonds (format: atom1</p> <p>Adding hydrogens...</p> <p>Idealizing hydrogen temperature factor...</p> <p>Finding het groups...</p> <p>Coloring atoms by element (green carbons in h</p> <p>done with preparation</p> <p>Writing to file...</p> |



Dialog - 3:50 - Postmortem (Diagnosis sum...)

File

Postmortem Flow Variables Job Manager Selection Memory Policy

Column containing JobId: S JobId

☒ Exclude structures

☒ Hide directory names when reporting files

Other args:

☐ Run postmortem for each row

OK Apply Cancel ?

Dialog - 3:47 - Job Control (View...)

File

Job Control | Flow Variables | Job Manager Selection | Memory Policies

Column containing JobId: [S] JobId

Actions: view Label for 'view' action: log

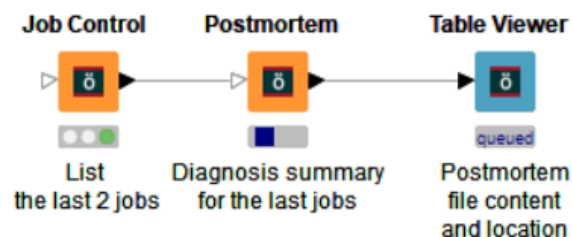
Flags

☐ children ☐ nochildren ☐ missing ☐ force

Query:

Other args:

OK Apply Cancel ?



| Row ID | S | ZipFile | Txt Output |
|--------|---|---|--|
| Row0 | | C:\Users\jcmozzic\AppData\Local\Temp\Postmortem_821843728\mhg-laptop-w26-0-5be046ca.zip | <pre> JobDB: C:\Users\jcmozzic\AppData\Local\Schrodinger\.jobdb2 archived C:\Users\jcmozzic\AppData\Local\Temp\Postmortem_821843728\mhg-laptop-w26-0-5be046ca.zip archived C:\Users\jcmozzic\AppData\Local\Temp\Postmortem_821843728\mhg-laptop-w26-0-5be046ca.zip * saved output of "C:\Program Files\Schrodinger2018-4\gxfinfo.exe" in file 'gxfinfo.log' * saved output of "C:\Program Files\Schrodinger2018-4\machid.exe" in file 'machid.log' </pre> |

Minor Improvements and Fixes

- The Run Canvas node takes sdf and smiles columns as input
- The parameter flow variable parsing of the Prime refine node is more robust
- Desmond MD node fixed to run on GPUs

Desmond trajectory manipulation copies all the simulation files

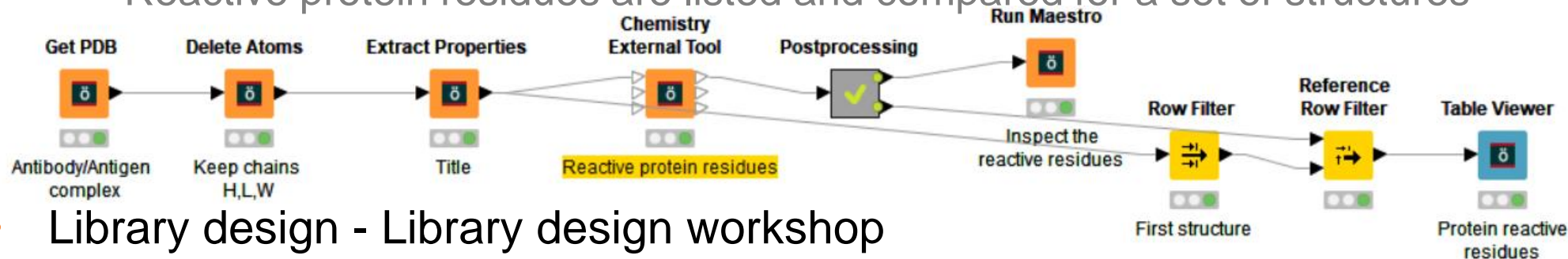
Chemistry external tool node fix to output Desmond trajectories

- The Setup diagnosis node outputs a warning in case of version mismatch

It is strongly recommended to link the extensions to the same release installation of the Schrodinger suite.

New and Improved Workflow Examples

- IO - LiveDesign
 - 3D structures are imported from LiveDesign
- Tools - Jobcontrol
 - Running the new Postmortem node. And the Jobcontrol node is used to view a calculation log
- Protein – Reactive protein residues
 - Reactive protein residues are listed and compared for a set of structures



- Library design - Library design workshop
 - Bioisostere and R-group enumeration using custom or predefined isosteres and libraries
 - Reaction-Based Enumeration to rapidly generate idea molecules with significant diversity and high probability of being synthesizable



New features in the KNIME extension

In Schrödinger Suite 2018-3

2018-3 New Features

- Includes the latest version of KNIME (v3.6.0)
 - except on Mac because of the size increase
- New **LiveDesign import and export** nodes
- New **Jobcontrol** node
- The Shape screening node optionally reports only the hit list
- The Glide ligand docking and Reaction-Based Enumeration nodes are more robust

[KNIME Schrödinger extensions version 4.3]

KNIME Analytics Platform 3.6- some new features

See details on the video

<https://tech.knime.org/whats-new-in-knime-36>,

and the full list of changes in the

<https://tech.knime.org/changelog-v36>

KNIME Workflow Hub

KNIME Analytics Platform

- Constant Value Column Filter
- Numeric Outliers
- Column Expressions
- Scorer (JavaScript)
- Usability Improvements
 - Connect/Unconnect nodes using keyboard shortcuts
 - Zooming

- Replacing and connecting nodes with node drop

- Call Workflow (Table Based)
- KNIME Server Connection
- Performance: Column Store (Preview)
- Making views beautiful: CSS changes
- KNIME Deep Learning, KNIME Big Data Extensions, Apache Kafka Integration, Text Processing, Git Nodes ...

KNIME Server

- Job View (Preview)
 - Look behind the scenes of a workflow running on KNIME Server
- Distributed Executors (Preview), Management (Client Preferences)

KNIME Analytics Platform 3.6- some new features

Dialog - 2:2 - Column Expressions

File

Formula

Flow Variables

Job Manager Selection

Memory Policy

+ -

↑ ↓

| Expression | Type | Replace Column | Output Column |
|---|---------------|-------------------------------------|---------------|
| capitalize(column("first_name")) | String | <input checked="" type="checkbox"/> | first_name |
| capitalize(column("last_name")) | String | <input checked="" type="checkbox"/> | last_name |
| a = column("age")if(isMissing(a)) a = 18if... | Boolean value | <input type="checkbox"/> | prediction |

Expression Editor

+ column

+ variable

+ function

```
1 a = column("age")
2
3 if(isMissing(a))
4   a = 18
5
6 if(and(a < 30, column("student"))) false
7 else true
```

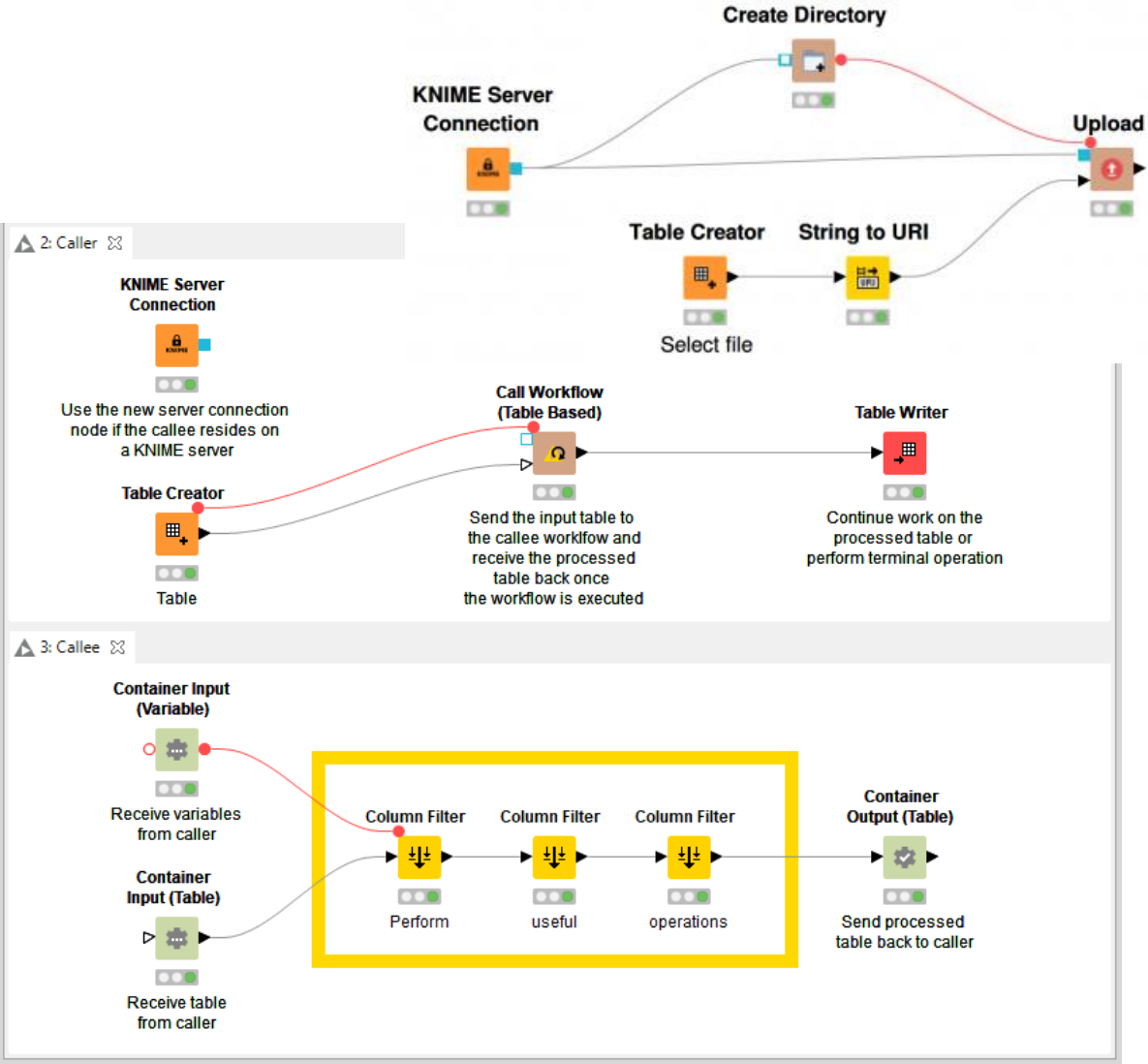
Scorer View

Confusion Matrix

| | false (Predicted) | true (Predicted) | |
|----------------|-------------------|------------------|---------|
| false (Actual) | 5872 | 0 | 100.0 % |
| true (Actual) | 24 | 6 | 20.0 % |
| | 99.6 % | 100.0 % | |

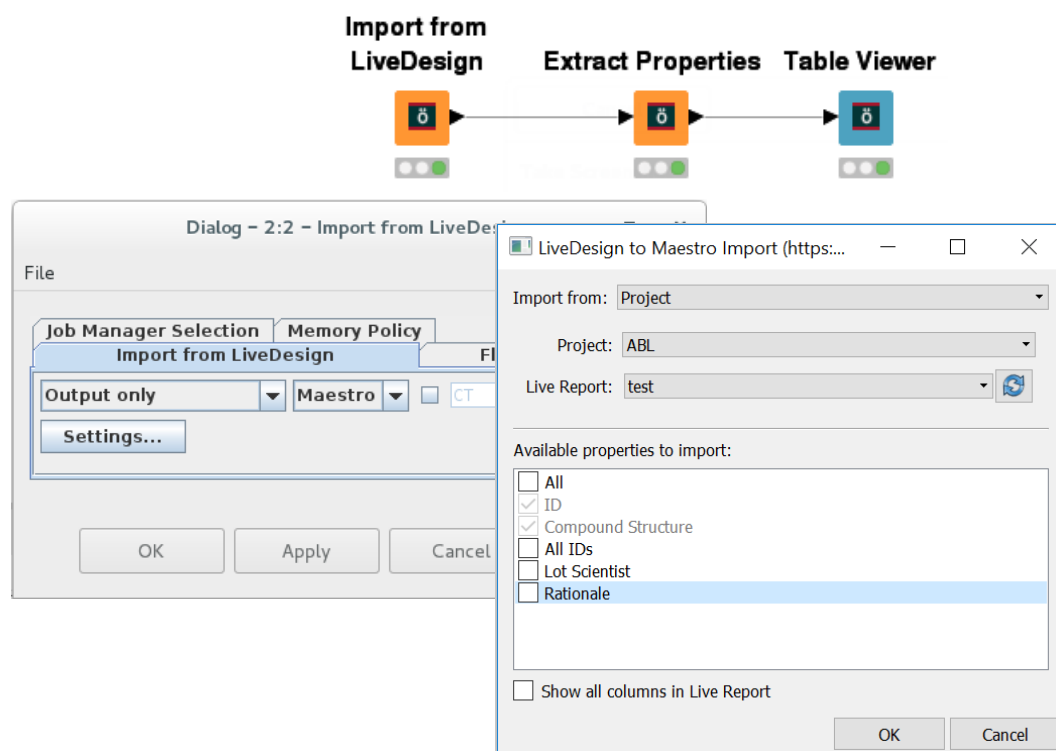
Overall Statistics

| Overall Accuracy | Overall Error | Cohen's kappa (κ) | Correctly Classified | Incorrectly Classified |
|------------------|---------------|-------------------|----------------------|------------------------|
| 99.6 % | 0.4 % | 0.332 | 5878 | 24 |



LiveDesign Import Node

- Using the same configuration panel as Maestro
 - Select the Project, LiveReport and the properties to import
 - Only 2D structures are imported for now

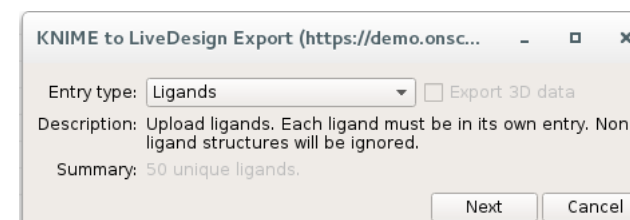
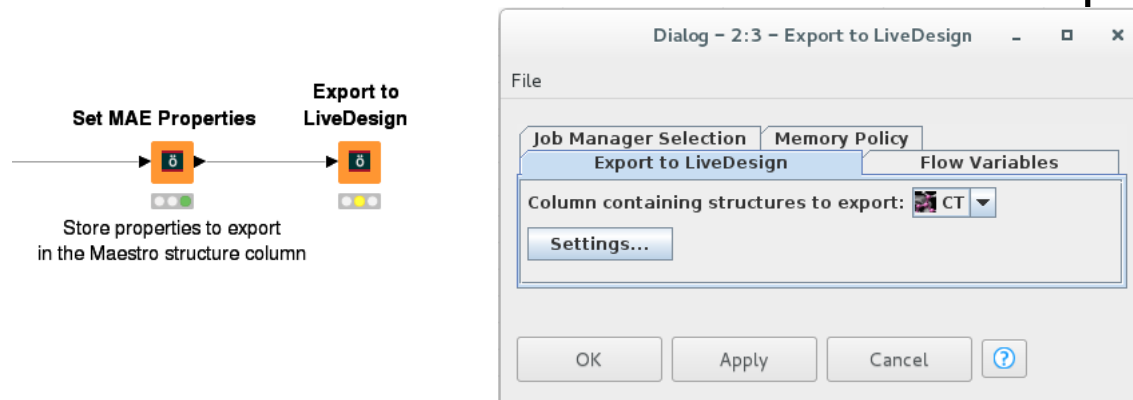


The screenshot shows the 'Table Viewer' window titled 'Extracted properties - 2:9 - Extract Properties'. It displays a table with 6 columns: 'Row ID', 'CT', '\$ All IDs', '\$ ID', '\$ Lot_Scientist', and '\$ Maestro...'. The table contains 35 rows of data, starting from Row0 to Row34. Each row represents a molecule entry with its ID, name, and associated scientist.

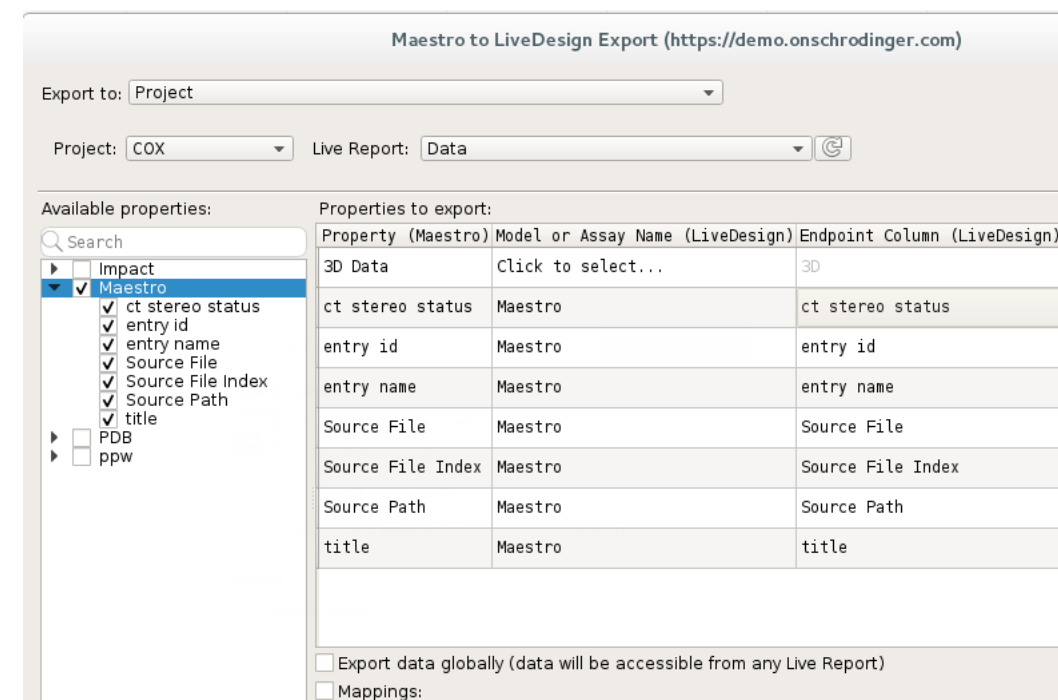
| Row ID | CT | \$ All IDs | \$ ID | \$ Lot_Scientist | \$ Maestro... |
|--------|------------------------------|------------|--------|---------------------|---------------|
| Row0 | Molecule: V83930 #atoms: ... | V83930 | V83930 | jean-christophe.... | 35 |
| Row1 | Molecule: V83931 #atoms: ... | V83931 | V83931 | jean-christophe.... | 141500 |
| Row2 | Molecule: V83932 #atoms: ... | V83932 | V83932 | jean-christophe.... | 151943 |
| Row3 | Molecule: V83933 #atoms: ... | V83933 | V83933 | ? | 165006 |
| Row4 | Molecule: V83934 #atoms: ... | V83934 | V83934 | ? | 177616 |
| Row5 | Molecule: V83935 #atoms: ... | V83935 | V83935 | ? | 184284 |
| Row6 | Molecule: V83936 #atoms: ... | V83936 | V83936 | ? | 193459 |
| Row7 | Molecule: V83937 #atoms: ... | V83937 | V83937 | ? | 290782 |
| Row8 | Molecule: V83938 #atoms: ... | V83938 | V83938 | ? | 334669 |
| Row9 | Molecule: V83939 #atoms: ... | V83939 | V83939 | ? | 399636 |
| Row10 | Molecule: V83940 #atoms: ... | V83940 | V83940 | ? | 400000 |
| Row11 | Molecule: V83941 #atoms: ... | V83941 | V83941 | ? | 403640 |
| Row12 | Molecule: V83942 #atoms: ... | V83942 | V83942 | ? | 412277 |
| Row13 | Molecule: V83943 #atoms: ... | V83943 | V83943 | ? | 451167 |
| Row14 | Molecule: V83944 #atoms: ... | V83944 | V83944 | ? | 504892 |
| Row15 | Molecule: V83945 #atoms: ... | V83945 | V83945 | ? | 527364 |
| Row16 | Molecule: V83946 #atoms: ... | V83946 | V83946 | ? | 534167 |
| Row17 | Molecule: V83947 #atoms: ... | V83947 | V83947 | ? | 550000 |
| Row18 | Molecule: V83948 #atoms: ... | V83948 | V83948 | ? | 563036 |
| Row19 | Molecule: V83949 #atoms: ... | V83949 | V83949 | ? | 564430 |
| Row20 | Molecule: V83950 #atoms: ... | V83950 | V83950 | ? | 582587 |
| Row21 | Molecule: V83951 #atoms: ... | V83951 | V83951 | ? | 591697 |
| Row22 | Molecule: V83952 #atoms: ... | V83952 | V83952 | ? | 600626 |
| Row23 | Molecule: V83953 #atoms: ... | V83953 | V83953 | ? | 644922 |
| Row24 | Molecule: V83954 #atoms: ... | V83954 | V83954 | ? | 647916 |
| Row25 | Molecule: V83955 #atoms: ... | V83955 | V83955 | ? | 672758 |
| Row26 | Molecule: V83956 #atoms: ... | V83956 | V83956 | ? | 687624 |
| Row27 | Molecule: V83957 #atoms: ... | V83957 | V83957 | ? | 700000 |
| Row28 | Molecule: V83958 #atoms: ... | V83958 | V83958 | ? | 702834 |
| Row29 | Molecule: V83959 #atoms: ... | V83959 | V83959 | ? | 710205 |
| Row30 | Molecule: V83960 #atoms: ... | V83960 | V83960 | ? | 716152 |
| Row31 | Molecule: V83961 #atoms: ... | V83961 | V83961 | ? | 726588 |
| Row32 | Molecule: V83962 #atoms: ... | V83962 | V83962 | ? | 732623 |
| Row33 | Molecule: V83963 #atoms: ... | V83963 | V83963 | ? | 755486 |
| Row34 | Molecule: V83964 #atoms: ... | V83964 | V83964 | ? | 766110 |

LiveDesign Export Node

- Select the Maestro structure column the properties should be exported from

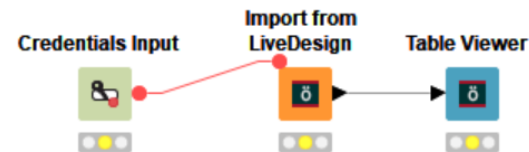


- Using the same configuration panel as Maestro
 - Select the Project, an existing LiveReport and the entry type
 - Choose the properties to export and the mapping



LiveDesign Nodes

- LiveDesign server
 - Saved once it has been configured
- Credentials
 - Saved during the session
 - as Workflow credential
 - in a Credential inputs quick form noc
 - or passed with the Use KNIME Server login option



Connect to LiveDesign

Please enter your credentials for LiveDesign

Host:

Username:

Password:

Workflow Credentials...

Edit Credentials for Workflow 'LD_Import_JC'.

| Name | Login | Password |
|-----------|------------------------------|----------|
| Id_import | Jean-christophe.mozziconacci | ***** |
| | | |
| | | |

Dialog - 0:11 - Credentials Input

File

Control Flow Variables Job Manager Selection Memory Policy

Label:

Description:

Variable Name:

Parameter Name:

Username:

Password:

☒ Prompt user name in wrapped metanode dialog/wizard

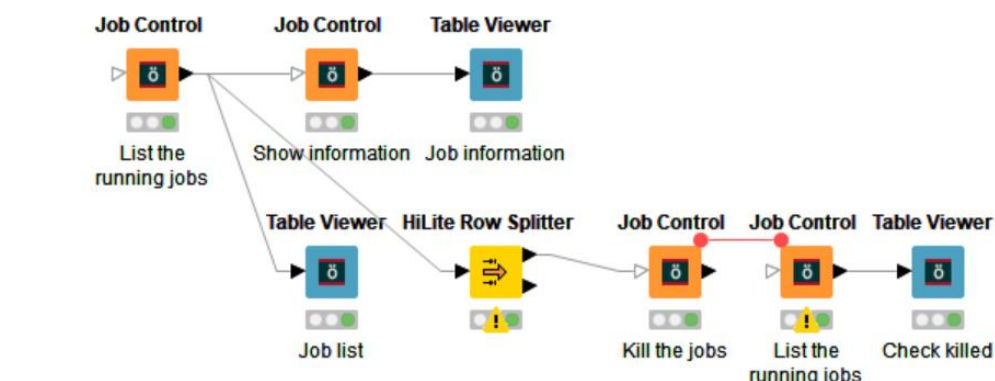
☐ Save password in configuration (weakly encrypted)

☒ Use KNIME Server Login (when run on server)

☐ Don't render input fields

Job control new node

- Action choice:
 - List completed or currently running calculations
 - Display information or list the job files
 - Kill some jobs
- Optionally operate on a column of Job IDs



| Table "default" - Rows: 3 Spec - Columns: 8 Properties Flow Variables | | | | | | | | |
|---|------------------------|------------|------------------------------|-----------|--------|--------------|------------|------------|
| Row ID | \$ JobId | \$ BatchId | \$ Name | \$ Status | \$ Err | \$ Time | \$ Runtime | \$ Host |
| Row0 | nyc-nx-l01-0-5b5c005f | | ReactionBasedEnum_1974090289 | running | | Jul-28 01:44 | 10m 02s | nyc-nx-l01 |
| Row1 | nyc-nx-l01-0-5b5c0295 | | AutoQSARBuild_1577104970 | running | | Jul-28 01:43 | 0m 05s | nyc-nx-l01 |
| Row2 | ^ nyc-nx-l01-0-5b5c... | | AutoQSARBuild_1577104970 | running | | Jul-28 01:44 | 0m 43s | nyc-nx-l01 |

| Row ID | \$ JobId | Txt JobInfo |
|--------|-----------------------|--|
| Row0 | nyc-nx-l01-0-5b5c005f | filesize: 4014 JobId: nyc-nx-l01-0-5b5c005f Name: ReactionBasedEnum_1974090289 Program: Combinatorial Synthesis Processors: 1 OrigLaunchHost: nyc-nx-l01.schrodinger.com OrigLaunchDir: /scr Host: nyc-nx-l01.schrodinger.com User: jcmozzic Dir: /scr HostsFile: /nfs/builds/NB/2018-3/2018-07-27/Linux-x86_64/schrodinger.hosts HostEntry: localhost Commandline: /nfs/builds/NB/2018-3/2018-07-27/Linux-x86_64/run_combinatorial_synthesis.py -out /scr/ReactionBasedEnum_1974090289.mae MmshareExec: /nfs/builds/NB/2018-3/2018-07-27/Linux-x86_64/mmshare-v4.3/bin/Linux-x86_64 JobHost: nyc-nx-l01.schrodinger.com JobUser: jcmozzic JobDir: /scr/jcmozzic/ReactionBasedEnum_1974090289 TmpDir: /scr JobDB: /home/jcmozzic/.schrodinger/.jobdb2 JobMmshareExec: /nfs/builds/NB/2018-3/2018-07-27/Linux-x86_64/mmshare-v4.3/bin/Linux-x86_64 JobPort: 46588 |

Job Control Flow Variables Job Manager Selection Mem

Column containing JobId:

Actions:

list

Flags

☐ children

☐ nochildren

☐ missing

☐ force

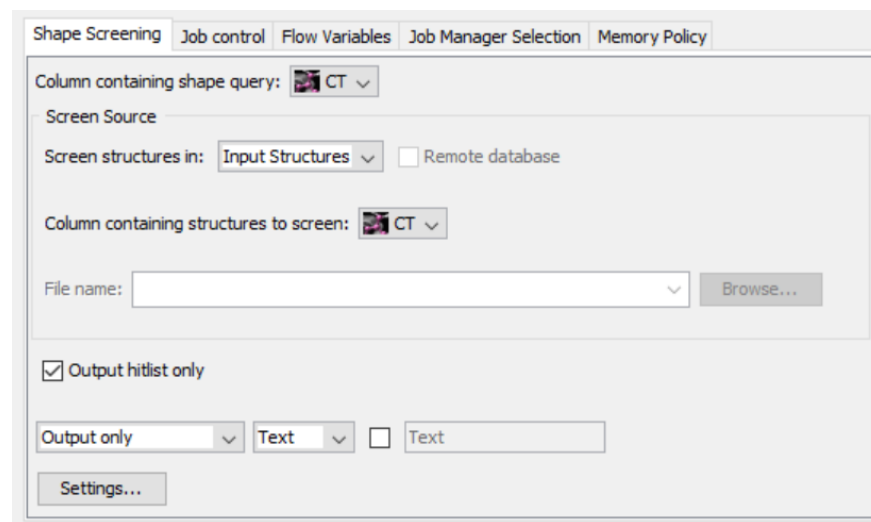
Query:

last1

Other args:

Minor Improvements and Fixes

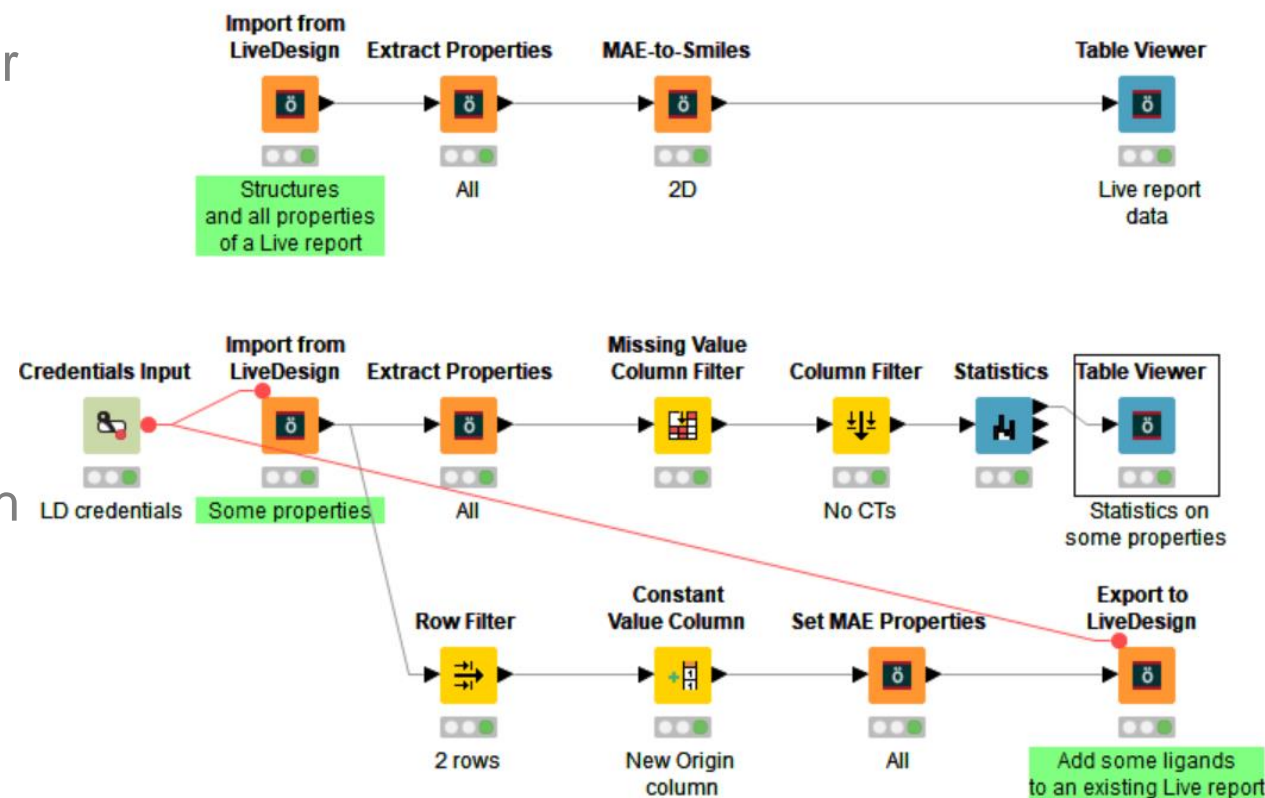
- The Shape screening node optionally reports only the hit list
Useful when screening or filtering a large database
And it reports the command run as flow variable



- The Glide ligand docking, Phase Screening and Reaction-based enumeration nodes are more robust

New and Improved Workflow Examples

- LiveDesign
 - New workflow under the General category
- Jobcontrol
 - New workflow under the Tools category
- Watermap metanode
 - Calculate for a set of structures in one sh
- Shape screening
 - Reporting only the hit list





New features in the KNIME extension

In Schrödinger Suite 2018-2

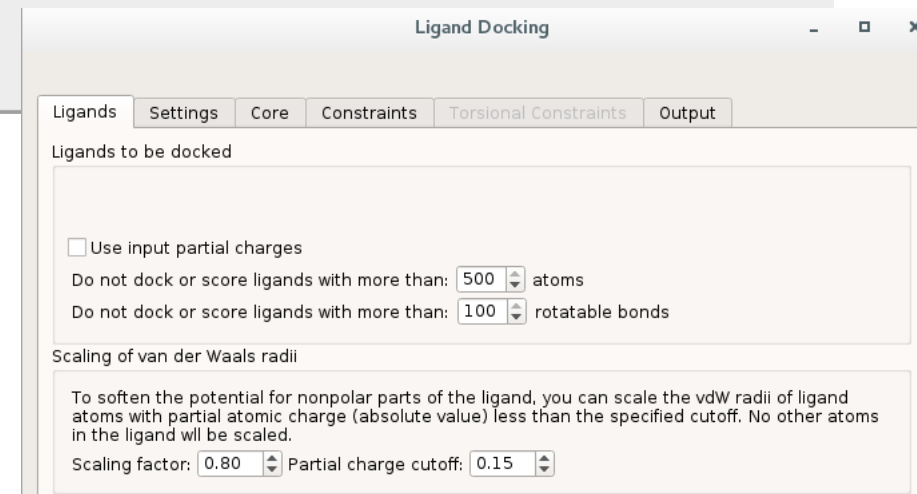
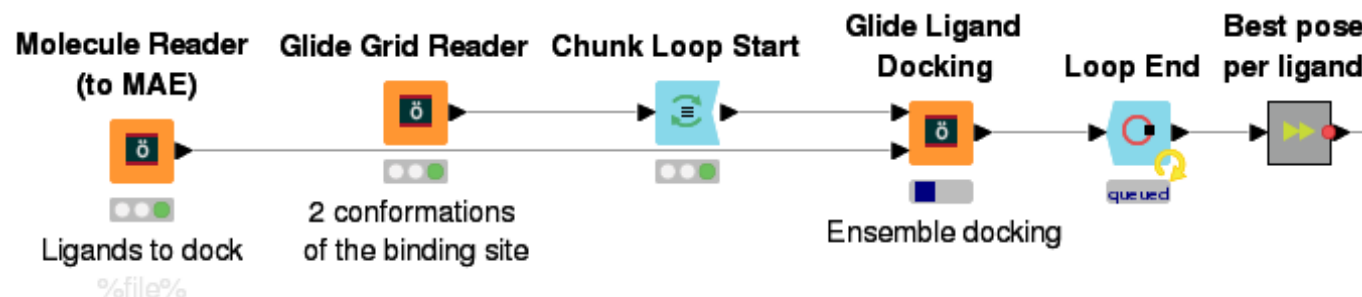
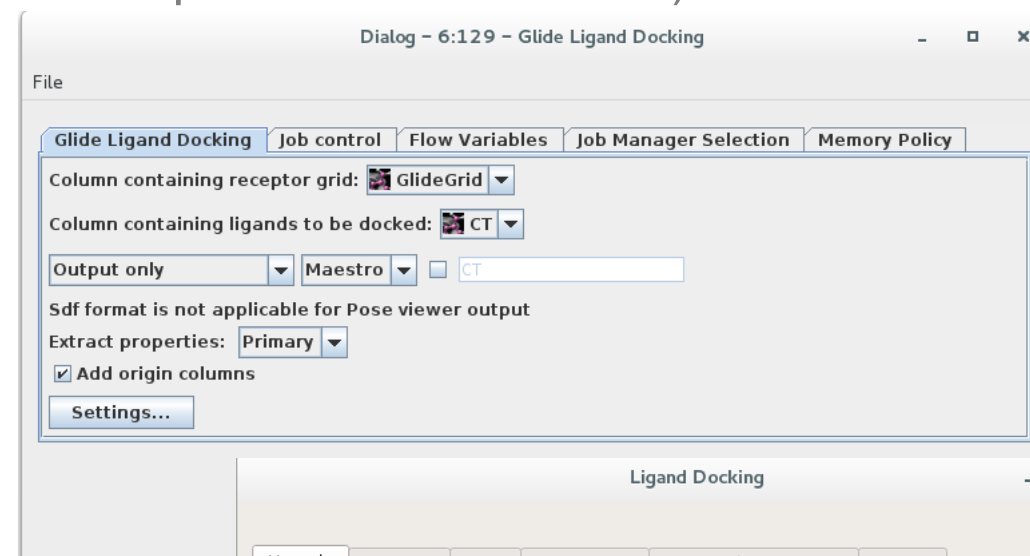
2018-2 New Features

- **Glide ligand docking** node has an updated **configuration panel**
- New **Reaction-based enumeration** node
- Includes the latest version of KNIME (v3.5.3)

[KNIME Schrödinger extensions version 4.2]

Glide Ligand Docking Node

- Node configuration with the same panel as in Maestro
 - It supports all constraints (including metal, NOE and positional constraints) except the torsional constraints
- It replaces the Ensemble docking node



Reaction Based Enumeration Node

- With the same panel as in Maestro
- In Labs category

- The node configuration is saved but not restored for now

Reaction-Based Enumeration

Review Pathways

Choose a pathway that will serve as the reaction.

Select a reaction pathway:

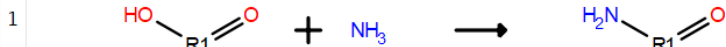
- Pathway 1
- Pathway 2
- Pathway 3
- Pathway 4

Reactions: 0 total, 0 shown

Filter Options...

Reactions

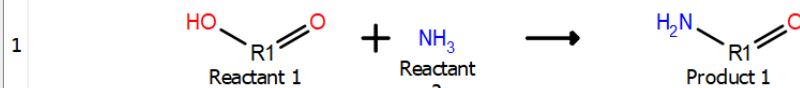
amide_coupling-1



Reaction-Based Enumeration

Reactant Setup

Reactions



Reactants

Define the reactants for the reaction.

Reactant 1

carboxylates (214385)

Reactant 2

amines-primsec (82156)

Options

Filter Options...

Maximum number of products: 10000

Reaction-Based Enumeration

Reaction Setup

Choose a single or multi-step reaction from a library, sketcher, or the PathFinder analysis of a compound.

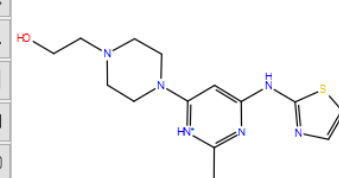
Get reaction from:

- ☒ PathFinder analysis
- ☐ Reaction library
- ☐ New sketch

Options:

Max depth: 1

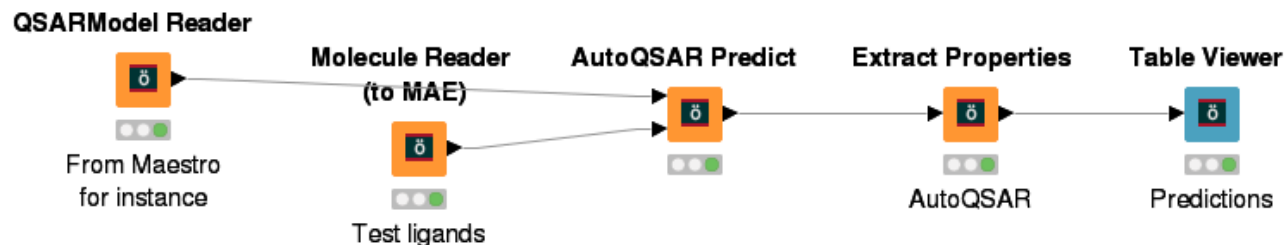
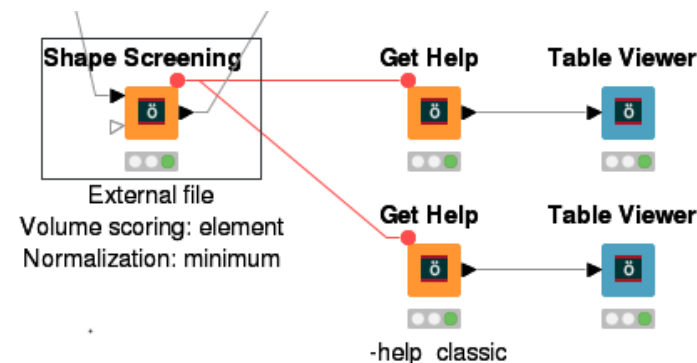
File Edit View



| Row ID | CT |
|--------|--------------------------------|
| Row0 | |
| Row1 | |
| Row2 | |
| Row3 | |
| Row4 | Molecule: 48579621 + 106499283 |
| Row5 | Molecule: 108094966 + 96407274 |
| Row6 | |
| Row7 | Molecule: 50489709 + 818627 |
| Row8 | Molecule: 42767631 + 38842934 |
| Row9 | Molecule: 81804186 + 114542574 |
| Row10 | Molecule: 50461353 + 35875298 |
| Row11 | Molecule: 108141326 + 96958549 |
| Row12 | Molecule: 31261023 + 1063713 |
| Row13 | Molecule: 95722968 + 107697448 |

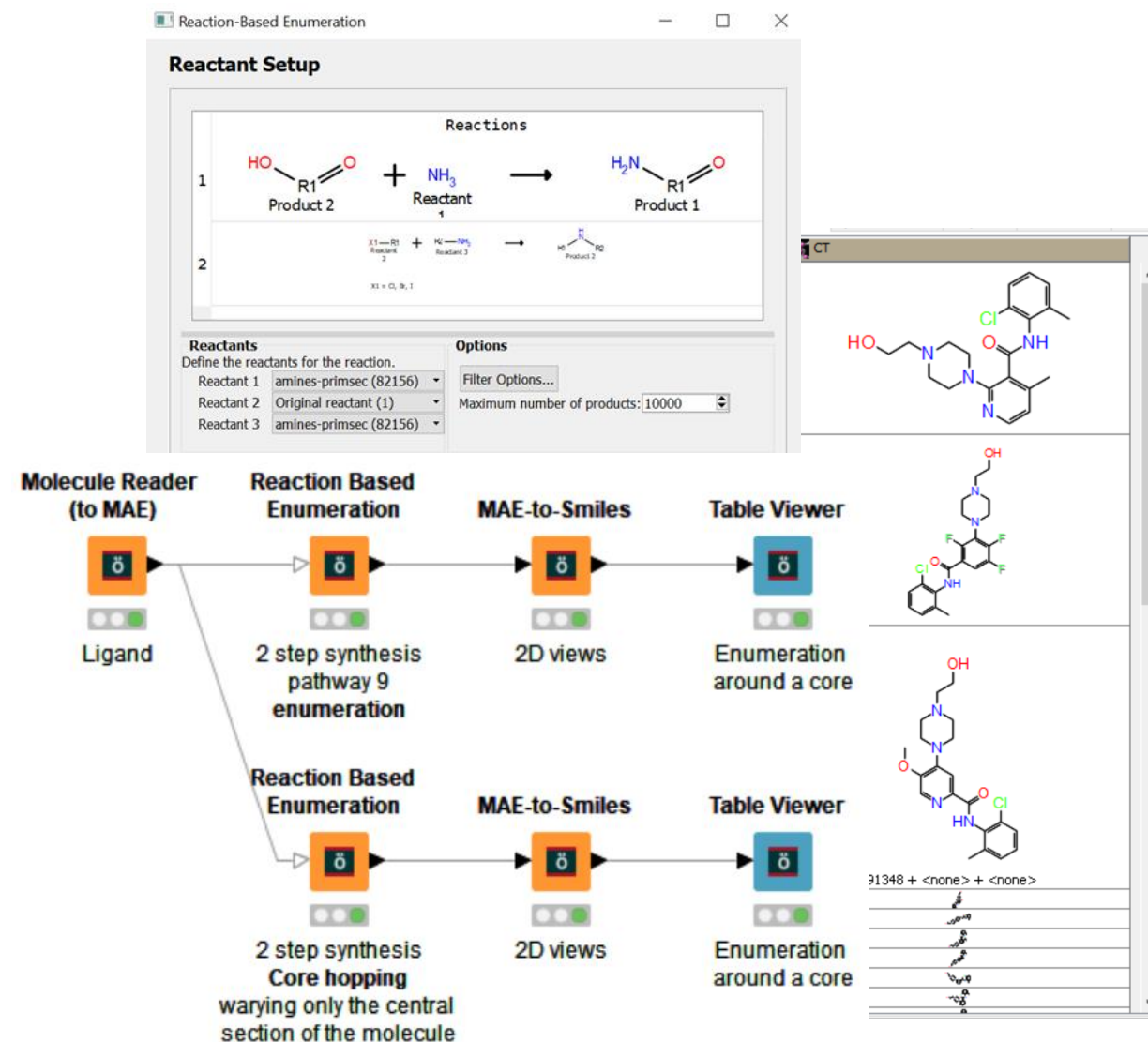
Minor Improvements and Fixes

- Run Maestro supports the new Phase hypothesis type
- Get Help node has an option field and is more robust
 - eg for `-help_classic` for Phase screening
- Extract Properties node is more robust on Windows
- Shape Screening and Phase DB creation configuration panel restoration is more robust
- New AutoQSAR model reader node



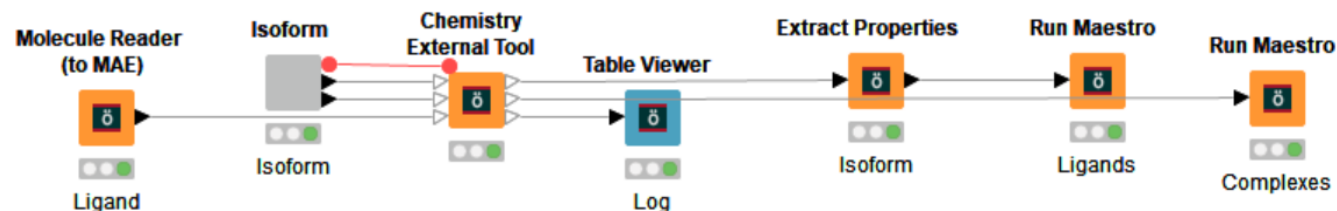
New and Improved Workflow Examples

- Reaction-based enumeration node
 - Use for enumeration and core hopping in a new workflow under Library design
- Glide ligand docking node
 - The new node is used in the relevant workflows, including the Ensemble docking workflow with the node in a loop
- AutoQSAR Reader node
 - In Cheminformatics – AutoQSAR



New and Improved Workflow Examples

- P450 Site of metabolism
 - New workflow under General category

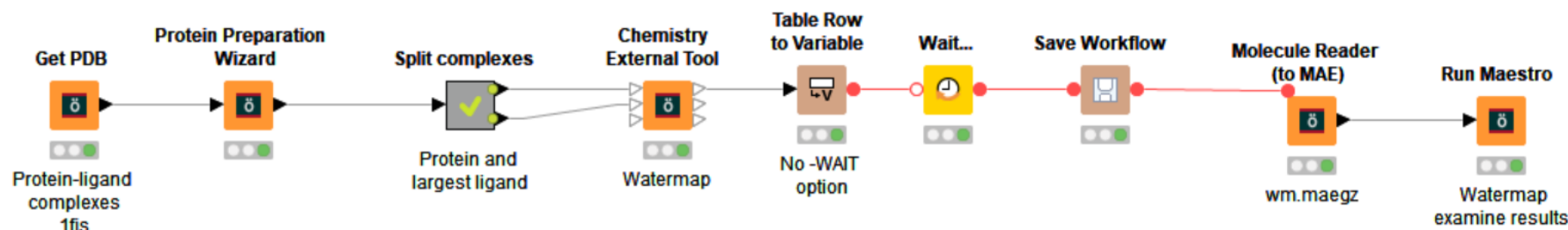


The QuickForms dialog box for the P450 Site of metabolism workflow. It has tabs for 'QuickForms', 'Flow Variables', 'Memory Policy', and 'Job Manager Selection'. The 'QuickForms' tab is active, showing the following settings:

- CYP Isoform: 2C9 (with a 'Change' checkbox)
- NUM_PRIME_CPUS: 4 (with a 'Change' checkbox)
- NUM_GLIDE_CPUS: 4 (with a 'Change' checkbox)

At the bottom, there are buttons for 'OK', 'Apply', 'Cancel', and a help icon.

- Watermap metanode
 - New Watermap workflow under Protein, where a Watermap job is submitted and the resulting map inspected in Maestro.



- Get help node
 - Pharmacophore – Shape screening and Labs – Parameter flow variable use-cases workflows



New features in the KNIME extension

In Schrödinger Suite 2018-1

2018-1 New Features

- Includes the latest version of **KNIME** (v3.5)
- New **Bioisoster replacement** node
- New Quick form nodes supported in KNIME workflows in Maestro
- **Antibody building, Sequence converter** metanodes
- Reduced the python panels (eg LigPrep node) opening time on Windows and 2D renderer speed up

[KNIME Schrödinger extensions version 4.1]

KNIME Analytics Platform 3.5 – Some New Features

- In Wrapped metanode, the node usage and layout in the KNIME portal is easier to control

Node

| | Row | Column | Width | |
|---|-----|--------|-------|--|
| Text Output ID: 10388 Description | 1 | 1 | 12 | |
| Column Selection ID: 9766 Cluster column | 2 | 1 | 6 | |
| String Input ID: 9767 Column name | 2 | 1 | 6 | |
| String Input ID: 10473 No suitable column | 4 | 1 | 12 | |
| Table View (JavaScript) ID: 10467 Table sample to help choosing the column5 lines | 5 | 1 | 12 | |
| Text Output ID: 10389 Next step | 6 | 1 | 12 | |
| Boolean Input ID: 10400 Activate the empty structure filtering step | 7 | 1 | 6 | |
| Boolean Input ID: 10392 Activate the Unique ID check step | 7 | 1 | 6 | |

Reset

Cluster column

Molecule

Column name

Cluster

Create a new column with:

| ity_2 ↑↓ | s_st_Chirality_3 ↑↓ | s_st_Chirality_4 ↑↓ | s_st_AtumChirality_1 ↑↓ |
|----------|---------------------|---------------------|-------------------------|
| | ? | ? | ? |
| | ? | ? | ? |
| | ? | ? | ? |
| | ? | ? | ? |
| | ? | ? | ? |

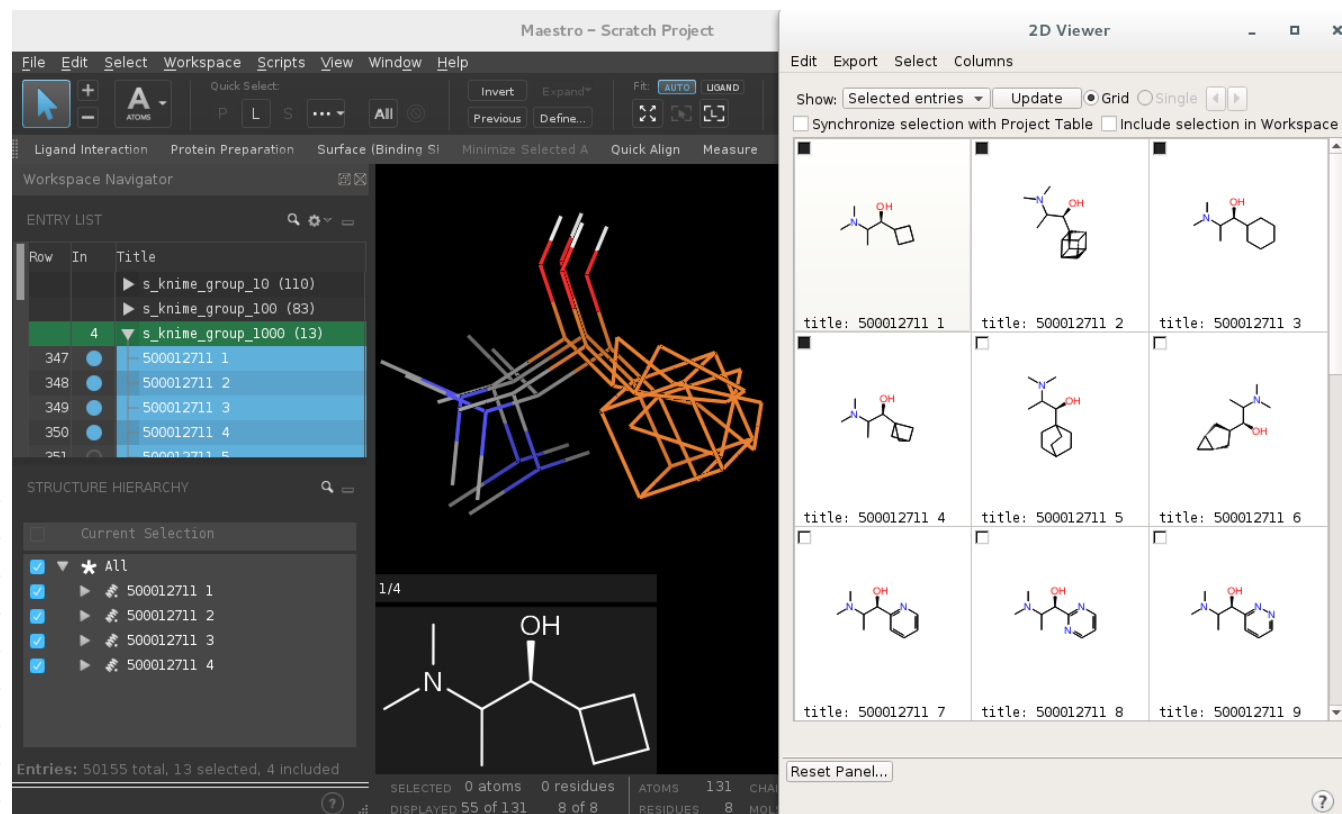
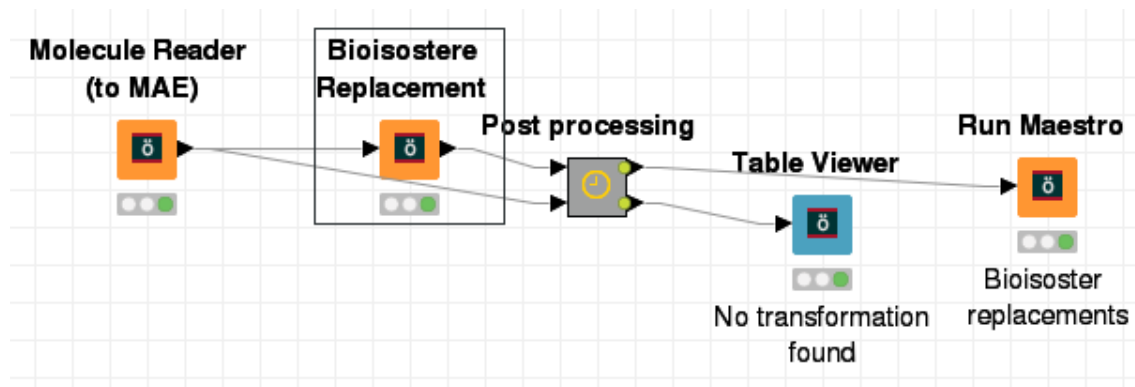
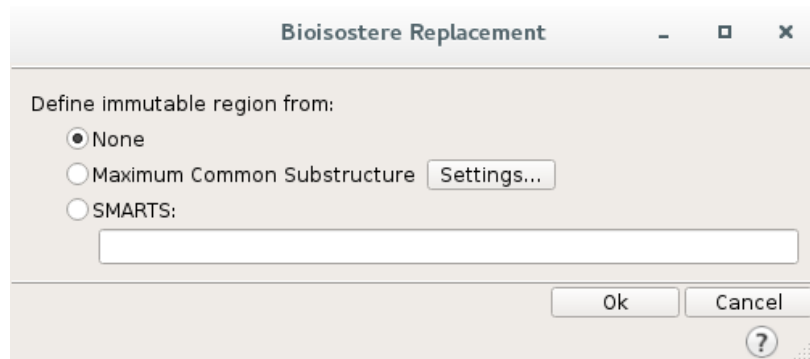
☒ Empty structure filtering

☐ Unique ID check

- With a standalone installation, waiting for KNIME 3.5.2 fix, the verbosity has to be changed in workspace

Bioisoster Replacement Node

- Node configuration with the same panel as in Maestro
- Under Library design



AutoQSAR – DeepChem

- New options available in the nodes using Maestro Python configuration pane
 - eg DeepChem method in the AutoQSAR node

AutoQSAR - Build model

Build model

Prediction property: Property type:

Options

Method: ☐ Traditional ☒ DeepChem (beta)

Random training set: Number of models to keep: [Advanced Options...](#)

Structures 50 total, 37 training, 13 test, 0 validation

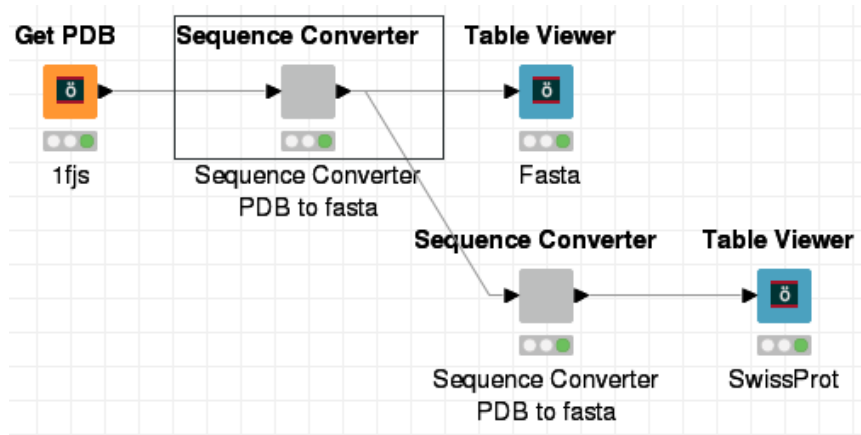
Ok Cancel

Minor Improvements and Fixes

- Performance improvements
 - Reduced the python panels (eg LigPrep node) opening time on Windows
 - 2D renderer speed-up
- Induced fit docking node configuration panel couldn't be restored between releases
- ConfGenX node robustness improvement
- KNIME-Maestro Connector node bugs
- New Quick form nodes supported in KNIME workflows in Maestro
 - To take advantage of the Wrapped metanodes

New and Improved Workflow Examples

- Sequence converter
 - New workflow under Protein category



- Bioisoster replacement
 - New workflow under Library design

Dialog - 2:14979 - Sequence Converter (Sequence Converter)

File

QuickForms Flow Variables Memory Policy Job Manager Selection

Input

Output

Start : read from this sequence in the input file

End : read to (and including) this sequence in the input file

Total : read at most this number of sequences

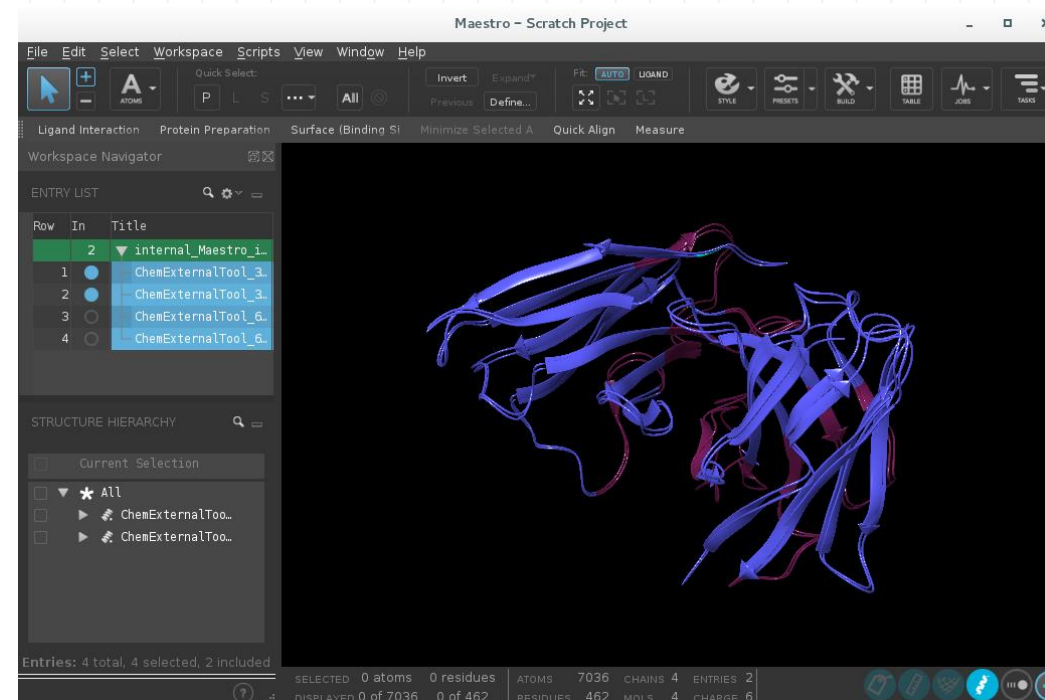
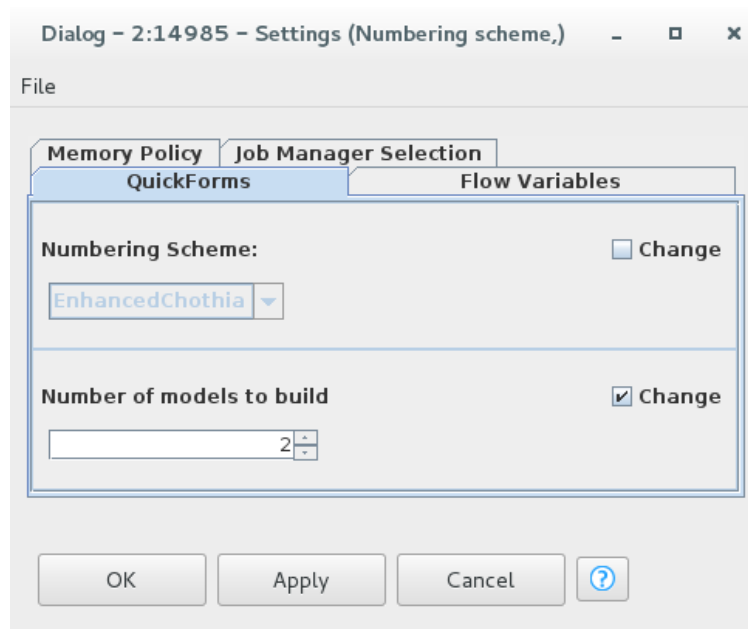
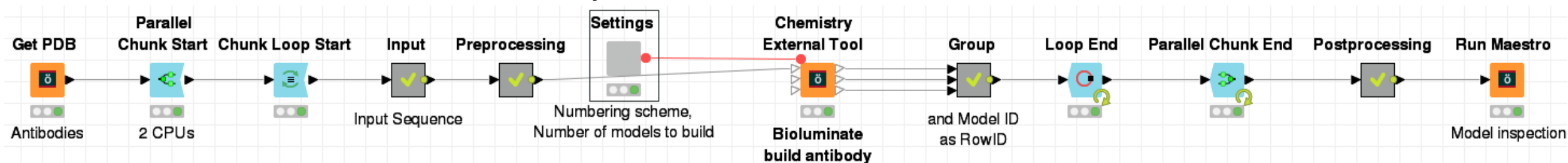
Read an alignment in the input file ☐

Use ATOM (not SEQRES) records with PDB files ☐

OK Apply Cancel ?

New and Improved Workflow Examples

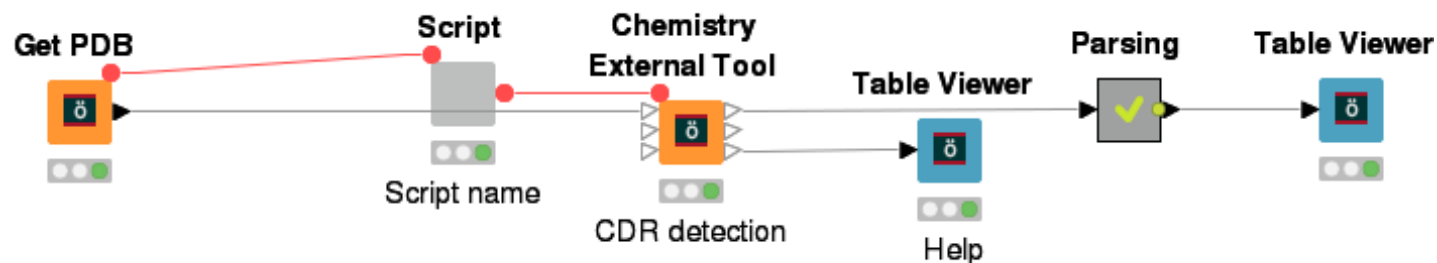
- Bioluminate Build antibody
- New workflow under Protein category



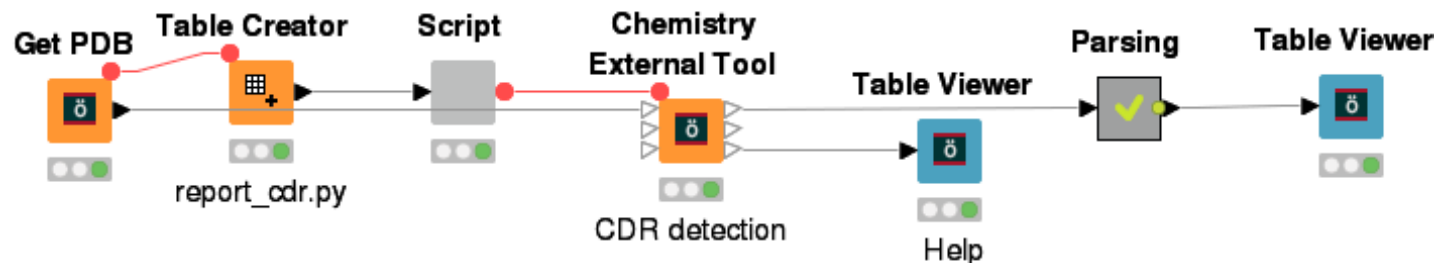
New and Improved Workflow Examples

- Python script execution (under General – Python)

A python script stored in the workflow in run in the Chemistry external tool node. The Python script can also be stored in the Table creator node to be edited easily



The python script run is embedded in the workflow. This makes easier to exchanges such workflows with colleagues.
Create the `knime://knime.workflow/Scripts` directory to store the "report_cdr.py" script in the workflow.



The script "report_cdr.py" is stored in the table creator node and can be edited easily.



New features in the KNIME extension

In Schrödinger Suite 2017-4

2017-4 New Features

- The Residue scanning, Conformer cluster and AutoQSAR nodes are more robust
- KNIME preferences can be changed and other option passed when run from Maestro

[KNIME Schrödinger extensions version 4.0]

KNIME preferences when run from Maestro or in batch

- When run from Maestro or in batch with KNIME_batch.py
 - Any KNIME batch or start-up script options (listed with knime -help) can be set in:
 - AppDataRoaming/Schrodinger/maestroxxx/KNIME.pref on Windows
 - .schrodinger/maestroxxx/KNIME.pref on Linux

eg -knimeInstallDir /path/newLocation/
-schrodingerTempDir /tmp/Schrodinger/
-maxHeap 1024m
-preferences=/path/file.epf
 - All the other KNIME preferences can be changed in the epf file specified above.

eg /instance/org.rdkit.knime.nodes/mcsAggregation.completeRingsOnlyOption=true
/instance/org.rdkit.knime.nodes/mcsAggregation.threshold=0.75
- In Maestro, Scripts, Install New Knime workflow
 - Since KNIME GUI is opened, the preferences have to be changed from File, Preferences or File, Import Preferences.



New features in the KNIME extension

In Schrödinger Suite 2017-3

2017-3 New Features

- Includes the latest version of **KNIME** (v3.4)
- New **Covalent docking** node
- New **Prime loop sampling** node
- New **Get Help** node
- **Desmond System Builder** and **Molecular Dynamics** nodes have updated configuration panels

[KNIME Schrödinger extensions version 3.9]

KNIME Analytics Platform 3.4 – Some New Features

- **KNIME Personal Productivity now part of KNIME Analytics Platform**

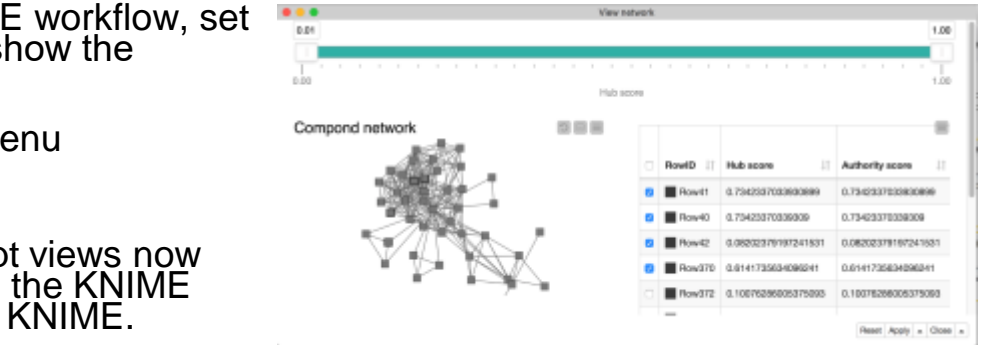
Now free Local Metanode templates, call local workflows inside of another KNIME workflow, set up your own version of KNIME's Workflow Coach, and use the Workflow Diff to show the differences between workflows or different versions of the same workflow.

Select 2 workflows in the KNIME explorer window and Compare in the pop-up menu

- **Wrapped metanode composite view**

The default view for wrapped metanodes containing quickforms and/or JavaScript views now shows the same view you would see if the wrapped metanode were opened with the KNIME Web Portal. This opens up many new possibilities for interactive data analysis in KNIME.

- Logistic Regression nodes are more scalable, faster and support regularization
- A new version of the Python integration
- New Date & Time integration
- Integration with the H2O machine learning library
- Audio and speech recognition nodes
- New JavaScript Views
- New Cloud Connectors



The screenshot shows a 'Workflow Comparison' window comparing two workflows. The top section lists the nodes in each workflow. The bottom section shows a 'Node Settings Comparison' table.

| Name | Type | Value |
|----------------------|---------|-------|
| hideInWizard | boolean | false |
| generateImage | boolean | true |
| showLegend | boolean | false |
| autoRange | boolean | true |
| useDomainInformation | boolean | false |
| showGrid | boolean | true |
| showCrosshair | boolean | false |
| snazToPoints | boolean | false |

KNIME Server 4.5: “Deploy to Server” and “Open in WebPortal” menu items

KNIME Big Data Extensions: Cloud connectors for common big data file formats, Support for Spark 2.0

See details on <https://tech.knime.org/whats-new-in-knime-34>, the video <https://www.youtube.com/watch?v=cex1xzq5OC8&feature=youtu.be>

and the full list of changes in the <https://tech.knime.org/changelog-v34>

Desmond System Builder and Molecular Dynamics

- Updated the types, tools and the node configuration dialog with the same panel as in Maestro

The image displays a workflow diagram and three dialog boxes from the Desmond software suite.

Workflow Diagram: A sequence of steps connected by arrows: **Get PDB** → **Protein Preparation Wizard** → **Desmond System Builder** → **Chemistry External Tool** (with a sub-note 'center.py') → **Desmond Molecular Dynamics** (with a sub-note 'Run Maestro') → **Desmond Trajectory Extract Frames** (with a sub-note 'All, no solvent nor counter ions'). A branch from 'Chemistry External Tool' leads to 'Inspect the system'.

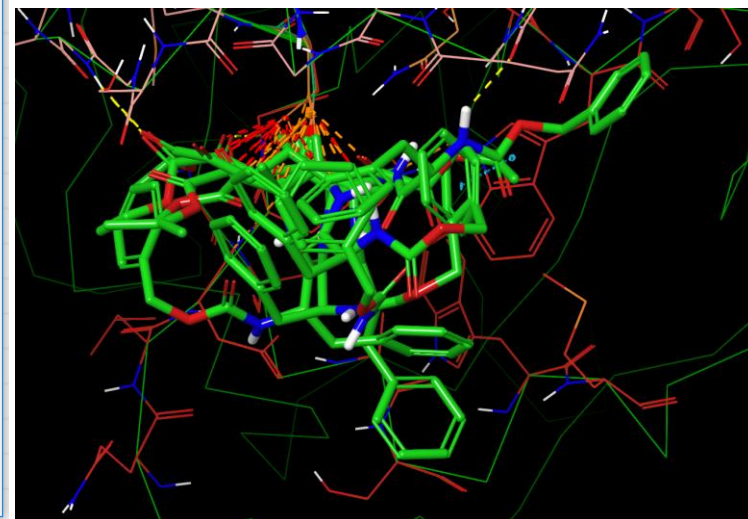
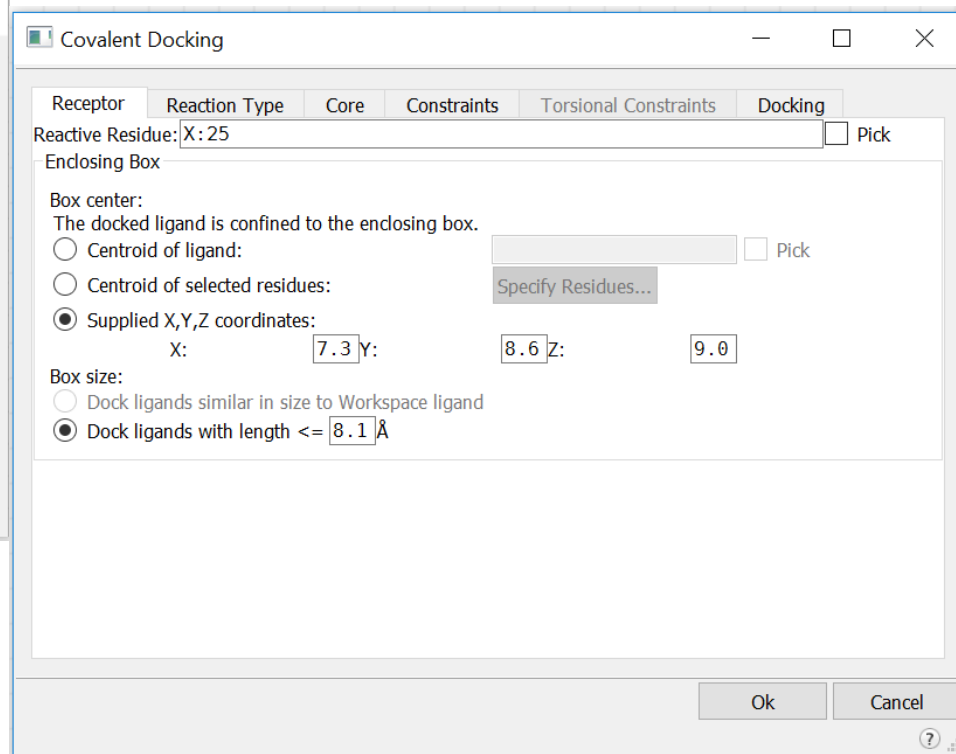
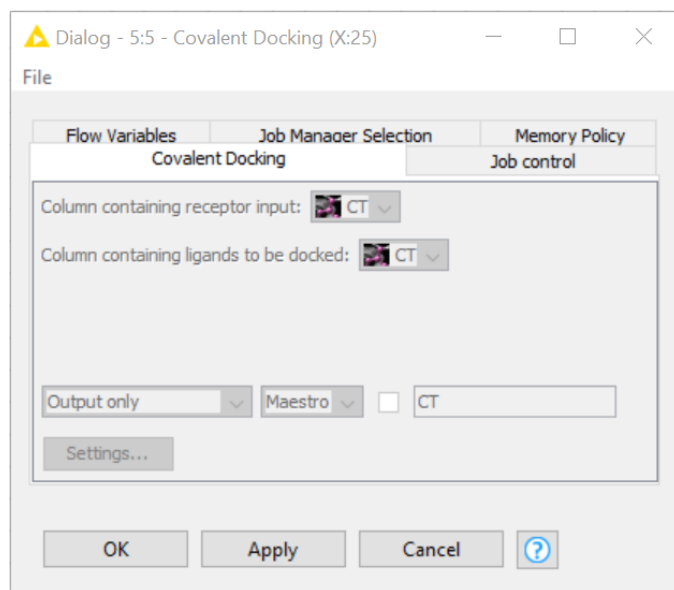
System Builder Dialog: Shows configuration options for the simulation environment. It includes tabs for 'Solvation' and 'Ions', a 'Set Up Membrane...' button, and a 'Delete Membrane' button. The 'Solvent model' section has radio buttons for 'None', 'Predefined: SPC' (selected), and 'Custom:'. The 'Boundary conditions' section includes a 'Box shape: Orthorhombic' dropdown, 'Box size calculation method' (radio buttons for 'Buffer' and 'Absolute size'), and input fields for 'Distances (Å): a: 10.0 b: 10.0 c: 10.0' and 'Angles (°): α: 90.0 β: 90.0 γ: 90.0'. The 'Box volume' is 248306 Å³. The 'Force field' is set to 'OPLS3'.

Dialog - 3:8391 - Desmond Molecular Dynamics: A configuration window for the molecular dynamics simulation. It includes a 'Model system' section stating 'SystemBuilder_1367178773_3-out (full system) contains 23705 atoms.' and a 'Simulation' section with fields for 'Simulation time (ns): total 0.012 elapsed 0.0', 'Recording interval (ps): trajectory 1.2 energy 0.12', 'Approximate number of frames: 10', 'Ensemble class: NPT', 'Temperature (K): 300.0', 'Pressure (bar): 1.01325', 'Surface tension (bar-Å) 0.0', and a checked 'Relax model system before simulation' option. It also has a 'Relaxation protocol' dropdown and a 'Browse...' button.

Dialog - 3:8390 - Desmond System Builder (Keep st...): A configuration window for the system builder. It includes tabs for 'Job Manager Selection', 'Memory Policy', 'Job control', and 'Flow Variables'. The 'Column containing input' is set to 'CMS'. The 'Output only' dropdown is set to 'CMS'. The 'Settings...' button is visible.

Covalent docking

- Node configuration with the same panel as in Maestro
- Under Docking and scoring:

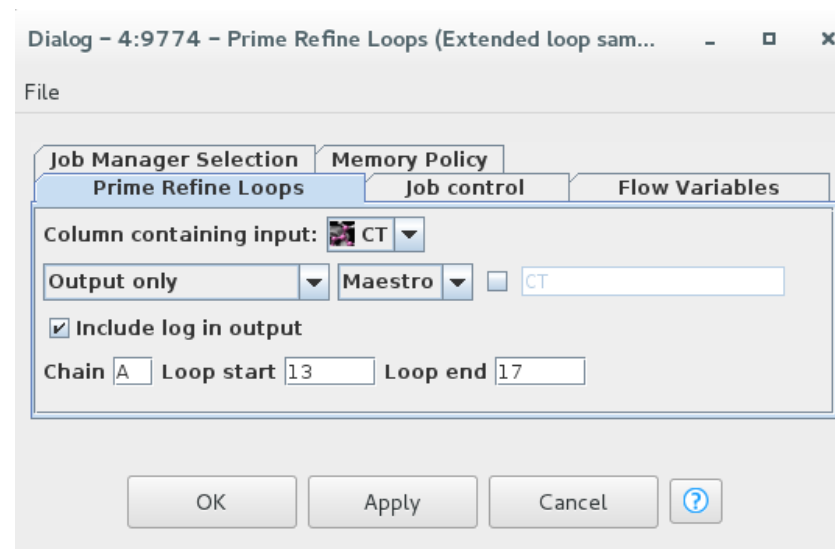
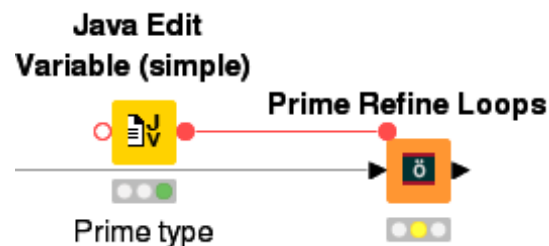


Prime loop sampling

- The node has a simplify configuration panel but all the GUI and command line options can be controlled through Parameter flow variables.

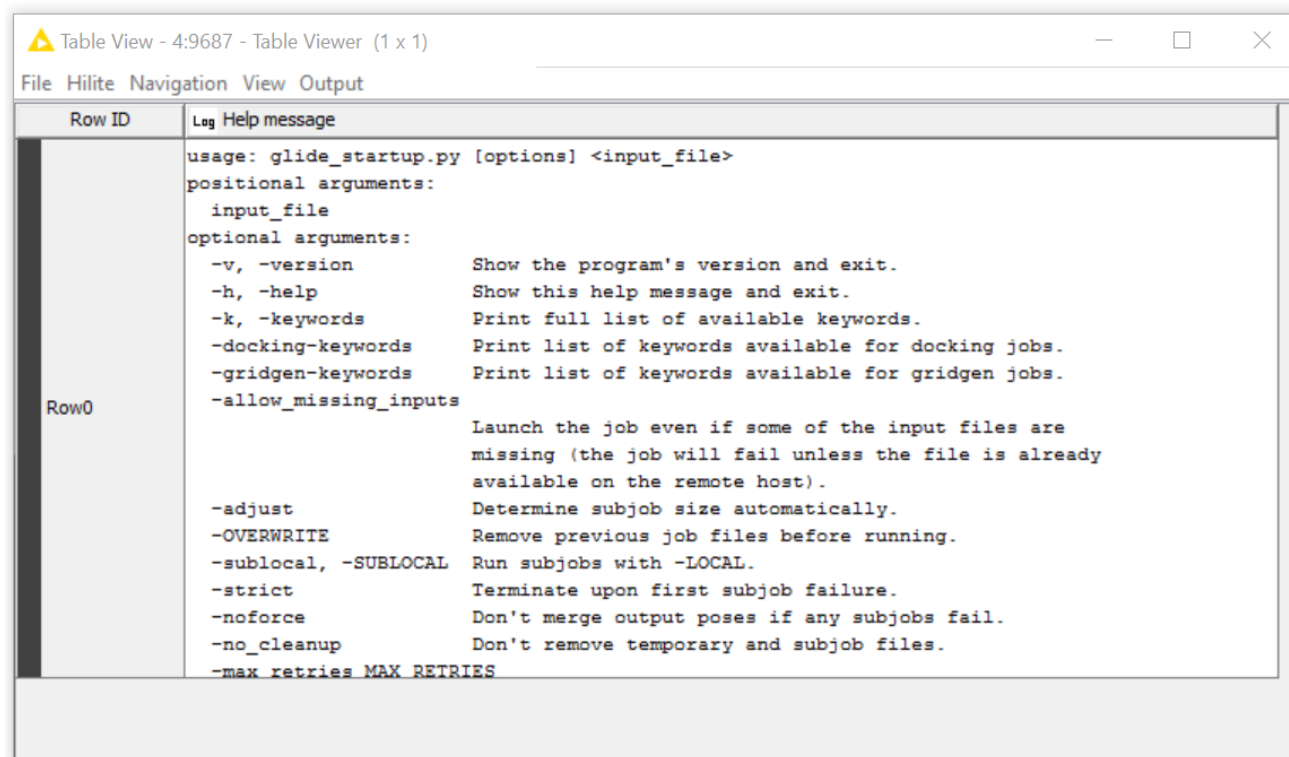
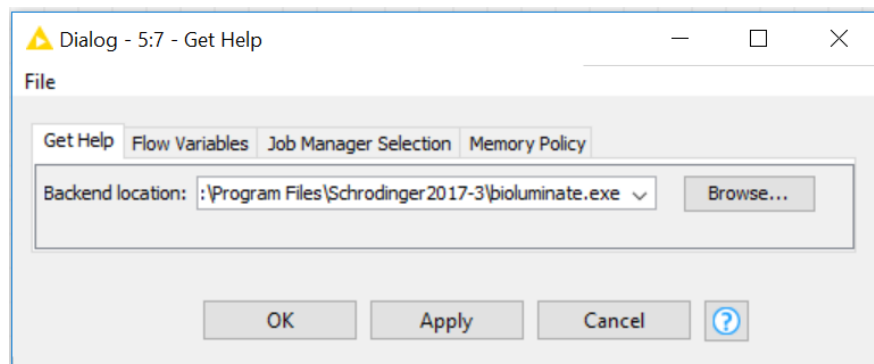
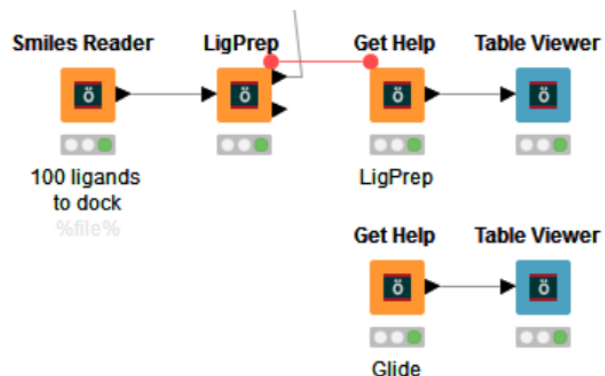
eg a string flow variable RefineLoops--PRIME_TYPE set to EXTENDED

See all the options in: https://www.schrodinger.com/sites/default/files/s3/mkt/Documentation/2017-3/docs/Documentation.htm#prime_command_reference/prime_commands_prime_input.htm



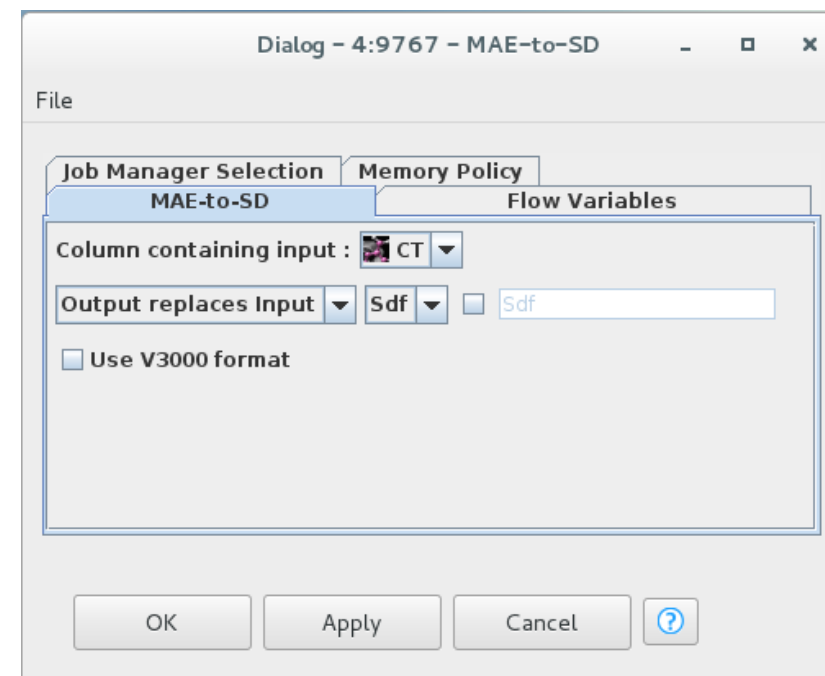
Get Help

- Shows command line options that can be passed through parameter flow variables
 - For a node (via the backend flow variable) or tool specified in the node.



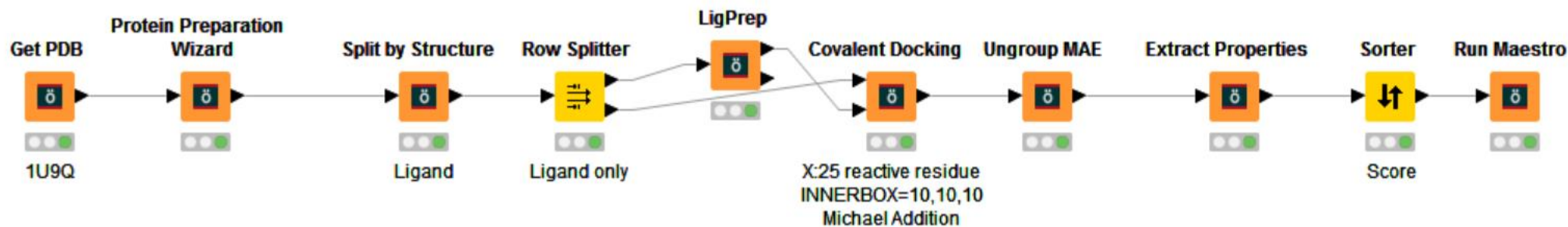
Minor Improvements and Fixes

- Mae-to-SD and SD-to_smiles nodes support V3000 format
- Extract properties supports the new Phase type as input
- Ligprep
 - Fixes in the new node, before removing the deprecated old node
- Chemistry External Tool- Sequence and Alignment properties not populated in Properties tab
- AutoQSAR Build Model
 - Error when executing the node with custom descriptors



New and Improved Workflow Examples

- Desmond System Builder and Molecular Dynamics
 - MD – MD simulation: updated workflows using the new nodes
- Covalent docking
 - Docking – Covalent docking: new workflow



- Prime loop sampling
 - Protein – Model building: additional branch using the new node and illustrating the Parameter flow variable control



New features in the KNIME extension

In Schrödinger Suite 2017-2

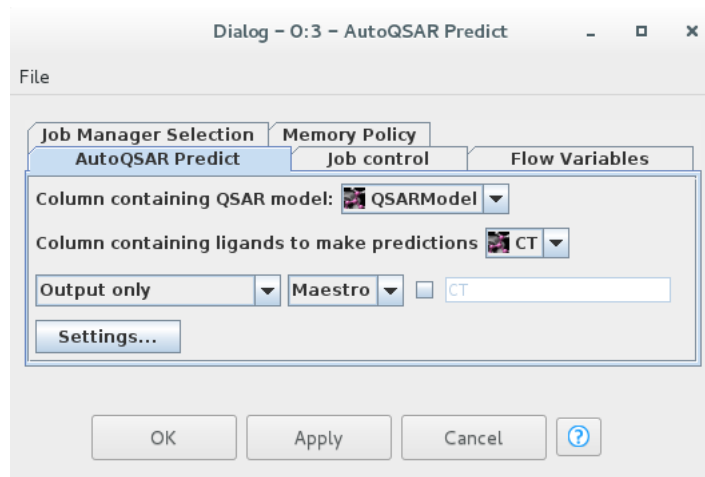
2017-2 New Features

- New **AutoQSAR** node
- Confgen node uses **Confgenx** fast 3D Conformation generator
- KNIME_batch.py takes .knwf workflow extensions
- Avoid confusing Potential deadlock in SWT display thread warning message in KNIME 3

[KNIME Schrödinger extensions version 3.8]

AutoQSAR node

- Node configuration with the same panel as in Maestro



AutoQSAR

Model Report

| Model Code | Score | S.D. | R ² | RMSE | Q ² | Q ² Min (Null Hypothesis) |
|--------------|--------|--------|----------------|--------|----------------|--------------------------------------|
| pls_23 | 0.7795 | 0.2834 | 0.8942 | 0.3377 | 0.8193 | -0.0615 |
| pls_14 | 0.7562 | 0.2876 | 0.8941 | 0.3508 | 0.7913 | -0.0006 |
| kpls_desc_24 | 0.7446 | 0.3043 | 0.8821 | 0.3624 | 0.7721 | 0.0212 |
| pls_24 | 0.7341 | 0.3202 | 0.8694 | 0.3734 | 0.7580 | 0.0212 |
| kpls_desc_23 | 0.7166 | 0.4396 | 0.7376 | 0.4311 | 0.7055 | -0.0615 |
| kpls_desc_19 | 0.6964 | 0.4059 | 0.7858 | 0.4241 | 0.6810 | 0.0750 |
| pls_19 | 0.6959 | 0.4189 | 0.7719 | 0.4292 | 0.6733 | 0.0750 |
| kpls_desc_14 | 0.6707 | 0.3845 | 0.8049 | 0.4297 | 0.6868 | -0.0006 |

Report Details... Show Less

Make Prediction

Model to test: All models (consensus prediction) Prediction property title: p_qp_QPlogBB

AutoQSAR Prediction: Y

Host=localhost:1, Incorporate=append

Ok Cancel

Report Details - kpls_desc_24

*
Report for Numeric Model kpls_desc_24

*

Ranking score = 0.744636

| Training Set | | Test Set | |
|--------------|----------------|----------|----------------|
| S.D. | R ² | RMSE | Q ² |
| 0.3043 | 0.8821 | 0.3624 | 0.7721 |

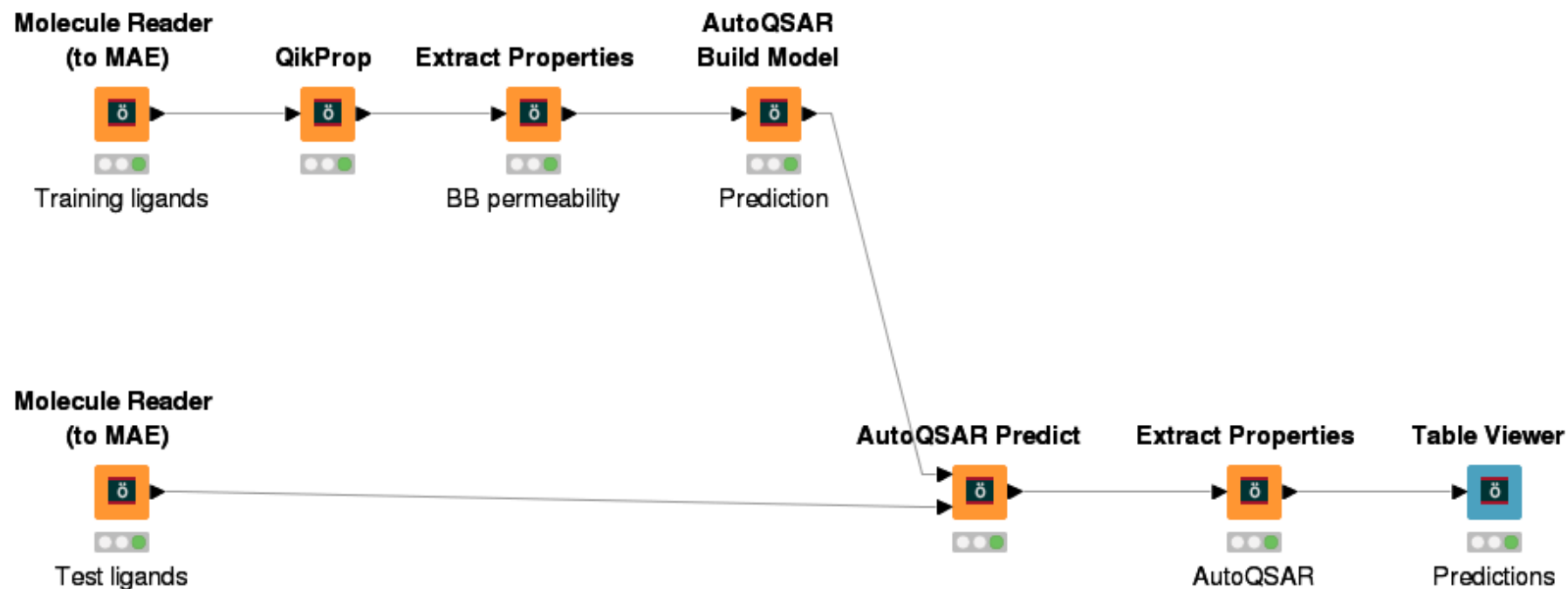
Optimum number of factors = 2

| ID Set | Y(Obs) | Y(Pred) | Error |
|----------|---------|---------|---------|
| 1 train | 0.1710 | 0.1283 | -0.0427 |
| 2 train | -0.3910 | -0.7082 | -0.3172 |
| 3 train | -0.0260 | -0.5846 | -0.5586 |
| 4 train | -1.3220 | -1.1265 | 0.1955 |
| 5 train | -0.1960 | -0.3488 | -0.1528 |
| 6 train | -1.4360 | -0.9411 | 0.4949 |
| 7 test | -1.3880 | -0.8562 | 0.5318 |
| 8 test | -0.3550 | -0.3829 | -0.0279 |
| 9 test | -1.3600 | -1.3285 | 0.0315 |
| 10 train | -0.1240 | -0.1800 | -0.0560 |
| 11 train | -1.4290 | -1.2630 | 0.1660 |
| 12 train | -1.1680 | -1.4022 | -0.2342 |
| 13 train | -2.0060 | -2.4324 | -0.4264 |
| 14 test | -1.5180 | -1.5796 | -0.0616 |
| 15 test | -0.9060 | -0.8116 | 0.0944 |
| 16 test | -1.1600 | -0.8606 | 0.2994 |
| 17 train | -1.5360 | -1.1857 | 0.3503 |
| 18 train | -0.5780 | -0.8591 | -0.2811 |
| 19 train | -1.3170 | -1.4563 | -0.1393 |
| 20 test | -1.9080 | -1.8081 | 0.0999 |
| 21 train | -0.7400 | -1.0074 | -0.2674 |
| 22 train | -1.7310 | -1.5502 | 0.1808 |
| 23 test | -0.7400 | -1.1097 | -0.3697 |
| 24 train | 0.3950 | 0.1005 | -0.2945 |
| 25 train | -0.1870 | -0.1018 | 0.0852 |
| 26 train | 0.4880 | 0.1833 | 0.3047 |

Scatter Plot... Se

New Workflow Example

- AutoQSAR node
 - Cheminformatics – AutoQSAR



2017-1 New Features

- Includes the latest version of **KNIME** (v3.3.1)
- LigPrep node has an updated configuration panel
- **Workflow list** node reports the script nodes and lists the flow variables controlling the node configuration
- **KNIME-Maestro Connector** node has a new **Phase Hypothesis mode**
- Chemistry External Tool node supports both Hypothesis formats

[KNIME Schrödinger extensions version 3.7]

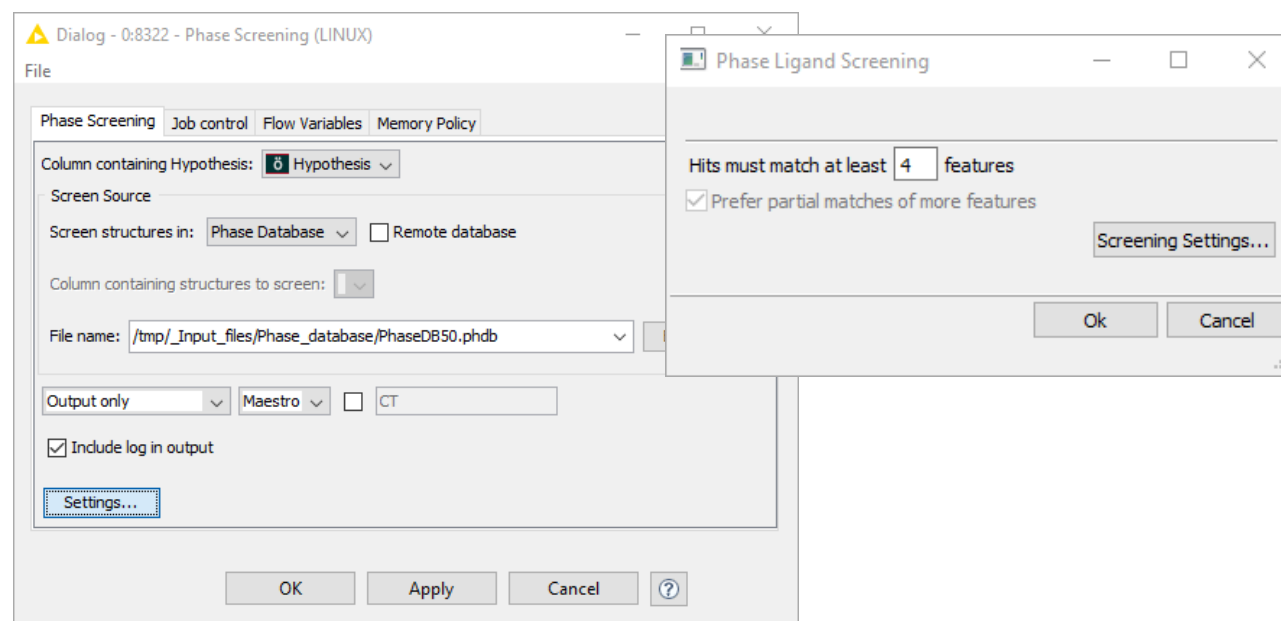
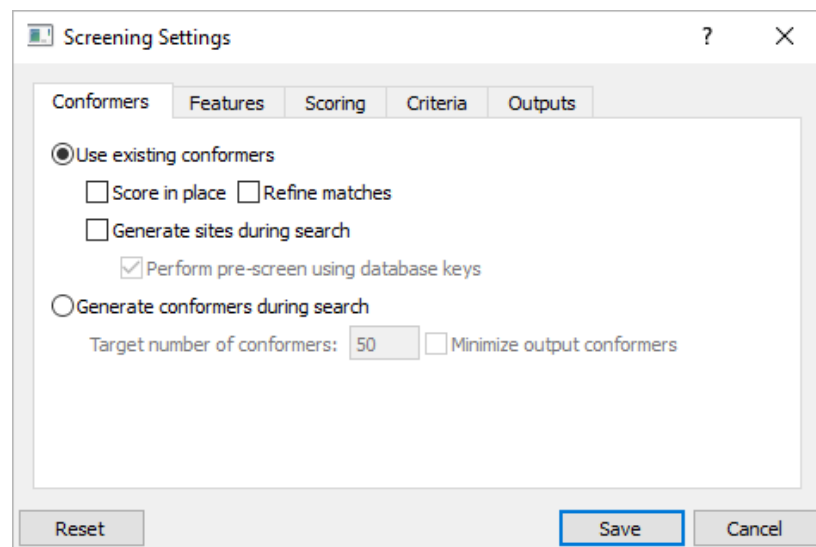
2016-4 New Features

- **Phase screening** node uses the new configuration panel and new algorithm
- **Any keyword** can be passed to the **Jaguar nodes**
- Extract properties node supports Sequence and Alignment inputs
- KNIME 3.x zipped update site is available in the installation

[KNIME Schrödinger extensions version 3.6]

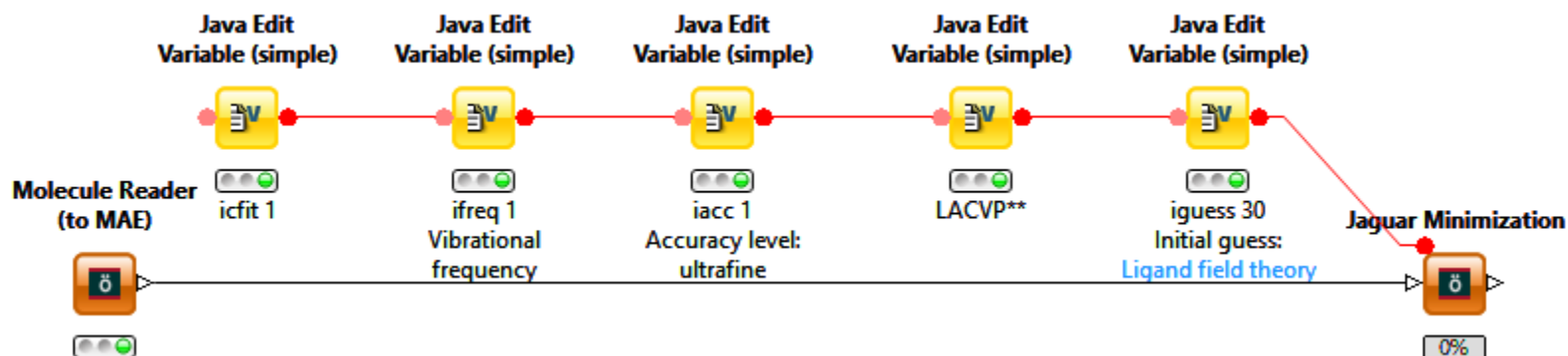
New Phase Screening Node

- Node configuration with the same panel as in Maestro
- The new node uses the new algorithm to screen compounds from Phase databases or files. Standard types (mae, sdf) are supported as input and output
- Phase Hypothesis Reader and Writer nodes support new (.phypo and .mae) and old (.xyz) Hypothesis formats



Jaguar and Extract Properties Nodes

- Any keyword can be passed as Parameter flow variable to the Jaguar nodes
 - eg INFO Jaguar Minimization Detected a JaguarMinimization flow variable: JaguarMinim-
-iguess=30



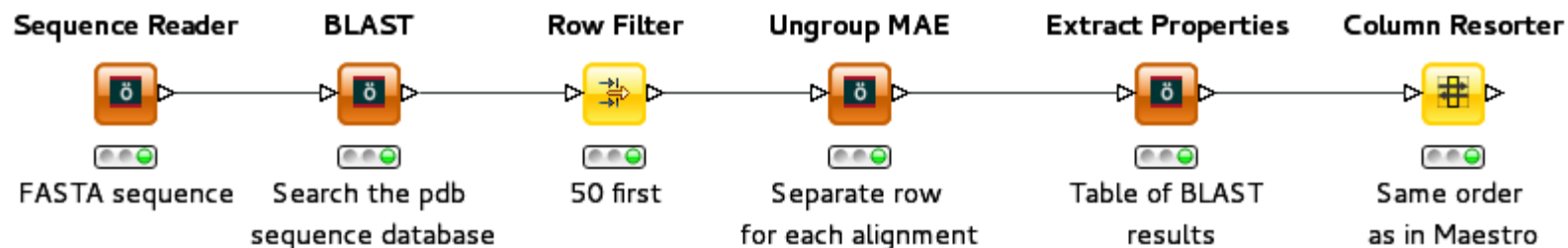
- Extract properties node supports Sequence and Alignment inputs

KNIME 3.x Zipped Update Site

- **KNIME 3.x compatible version**
 - The zipped update site available is in the installation under `$SCHRODINGER/knime-v*/data/`
(along with the KNIME 2.12 version)

Improved Workflow Examples

- Phase screening
 - Pharmacophore – Phase screening: use the new node
 - Same node for Phase database and file screening
- Extract properties supports Sequence and Alignment inputs
 - Protein – Model building: chose alignments in a list with corresponding properties



| Table View - 14:120 - Table Viewer (Inspect the possible) | | | | | | | | | | |
|---|--------------------------|------------|--|------------|----------------------|----------------|----------------------|--------------------------|---------------|------------------------|
| File | Hilite | Navigation | View | Output | | | | | | |
| Row ID | Alignment | I align... | S seq_description | S seq_n... | I align_end_position | D align_evalue | I align_percent_gaps | I align_percent_positive | D align_score | I align_start_position |
| Row447 | Alignment: #sequences... | 98 | gi 448262480 pdb 4E0M C Chain C, Thr 160 Phosphorylated Cdk2 H84s, Q... | 4E0M_C | 297 | 0 | 0 | 98 | 1,561 | 1 |
| Row448 | Alignment: #sequences... | 98 | gi 448262470 pdb 4E0K A Chain A, Thr 160 Phosphorylated Cdk2 H84s, Q... | 4E0K_A | 297 | 0 | 0 | 98 | 1,560 | 1 |
| Row449 | Alignment: #sequences... | 98 | gi 448262472 pdb 4E0K C Chain C, Thr 160 Phosphorylated Cdk2 H84s, Q... | 4E0K_C | 297 | 0 | 0 | 98 | 1,560 | 1 |
| Row450 | Alignment: #sequences... | 98 | gi 448262474 pdb 4E0L A Chain A, Thr 160 Phosphorylated Cdk2 H84s, Q... | 4E0L_A | 297 | 0 | 0 | 98 | 1,560 | 1 |
| Row451 | Alignment: #sequences... | 98 | gi 448262476 pdb 4E0L C Chain C, Thr 160 Phosphorylated Cdk2 H84s, Q... | 4E0L_C | 297 | 0 | 0 | 98 | 1,560 | 1 |
| Row452 | Alignment: #sequences... | 99 | gi 149242354 pdb 2JGZ A Chain A, Crystal Structure Of Phospho-Cdk2 In C... | 2JGZ_A | 288 | 0 | 0 | 99 | 1,531 | 1 |
| Row453 | Alignment: #sequences... | 64 | gi 822599530 pdb 4YC6 A Chain A, Cdk1/cks1 | 4YC6_A | 296 | 0 | 3 | 78 | 1,044 | 1 |
| Row454 | Alignment: #sequences... | 64 | gi 822599532 pdb 4YC6 C Chain C, Cdk1/cks1 | 4YC6_C | 296 | 0 | 3 | 78 | 1,044 | 1 |
| Row455 | Alignment: #sequences... | 64 | gi 822599534 pdb 4YC6 E Chain E, Cdk1/cks1 | 4YC6_E | 296 | 0 | 3 | 78 | 1,044 | 1 |
| Row456 | Alignment: #sequences... | 64 | gi 822599536 pdb 4YC6 G Chain G, Cdk1/cks1 | 4YC6_G | 296 | 0 | 3 | 78 | 1,044 | 1 |
| Row457 | Alignment: #sequences... | 62 | gi 158430247 pdb 2OKR A Chain A, Cryptosporidium Parvum Cyclin-Depend | 2OKR_A | 289 | 0 | 1 | 81 | 975 | 1 |

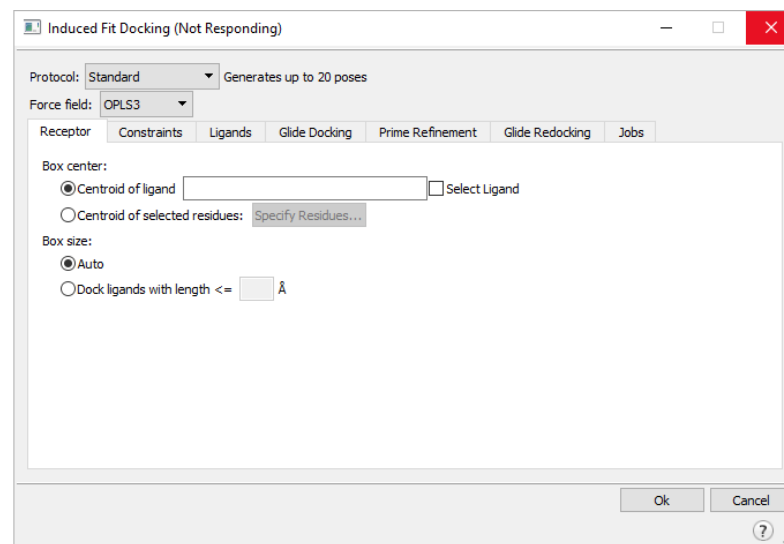
2016-3 New Features

- **KNIME 3.x** is officially supported
(separate zipped and update site version compatible)
- **Induced fit docking** has an updated configuration panel
- In **Maestro 11**:
 - Establish structure exchange with KNIME moved to Tasks > Workspace and Project table operations > KNIME
 - The workflow menu has been merged with the Script menu

[KNIME Schrödinger extensions version 3.5]

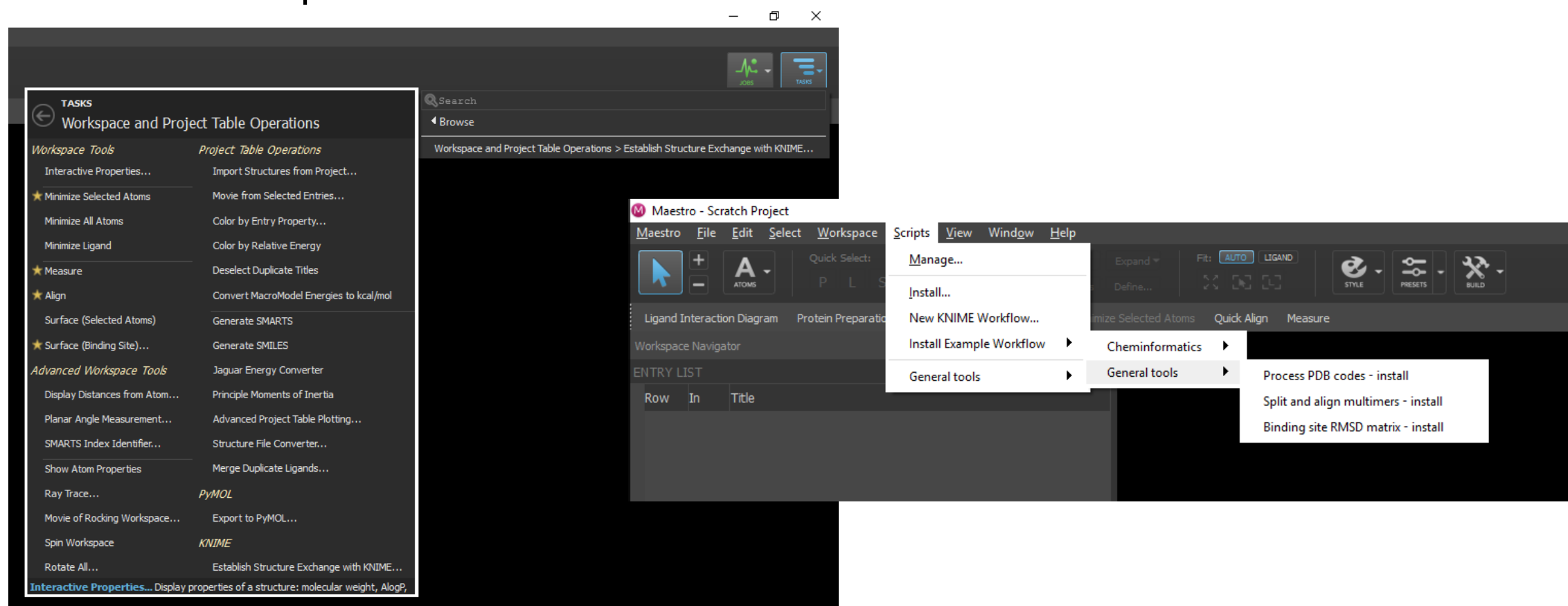
KNIME 3.x and Induced fit docking node

- KNIME 3.x is officially supported
 - Specific versions available on the update site The nodes supporting mol2 and sdf input and output adapter cells
- Induced fit docking node
 - Updated node configuration with the same panel as in Maestro



KNIME menus in Maestro 11

- Establish structure exchange with KNIME has been moved to Tasks > Workspace and Project table operations > KNIME
- The workflow menu has been merged with the Script menu where KNIME workflows can now be imported and run in Maestro



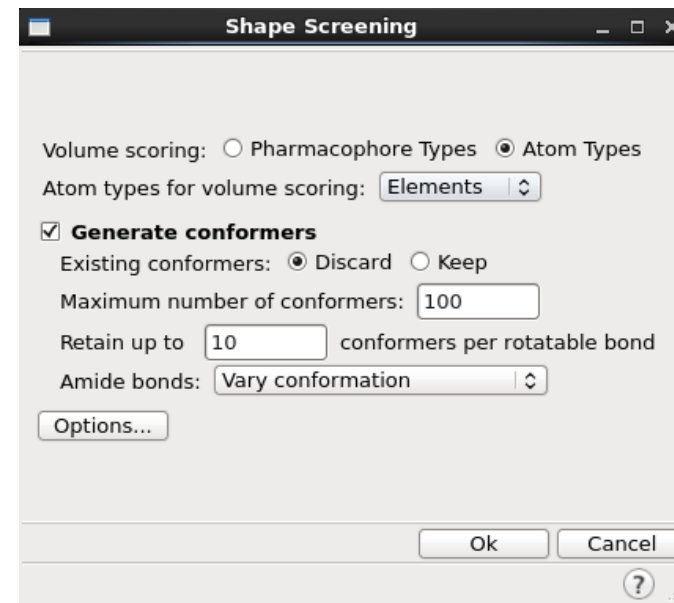
2016-2 New Features

- Minor improvements in the **Shape Screening** node
- The **Python Script** nodes pass unsupported types to the output table
- Fixed output column row matching when some rows are missing
- Minor improvements in the Extract Atom/bond Properties node

[KNIME Schrödinger extensions version 3.4]

New features

- Shape screening
 - Minor improvements and the new version of the node has been moved to the Pharmacophore modeling category
- Python Script nodes
 - Pass unsupported types to the output table
- Fixed output column row matching when some rows are missing
 - eg failed structures, “duplicate row ID” error message
- Minor improvements in the Extract Atom/bond Properties node
 - Handle missing input cells, Populate the Properties tab in output tables



2016-1 New Features

- Still includes KNIME 2.12 but a KNIME 3.1 compatible version is available for testing
- **Shape screening** has an updated configuration panel and URLs are supported
- The **parameter flow variables** can be used in Strain Rescore node and more Canvas nodes
- Short property names and Include input available in the Extract Atom/bond Properties node

[KNIME Schrödinger extensions version 3.3]

KNIME 3.1- some New Features

- **GUI and general Structure**

- New Look and Feel, New Eclipse and Java (Java 8, Eclipse 4, and BIRT 4)
- WrappedNodes
- Node Repository - Fuzzy Search

- **Analytics and ETL**

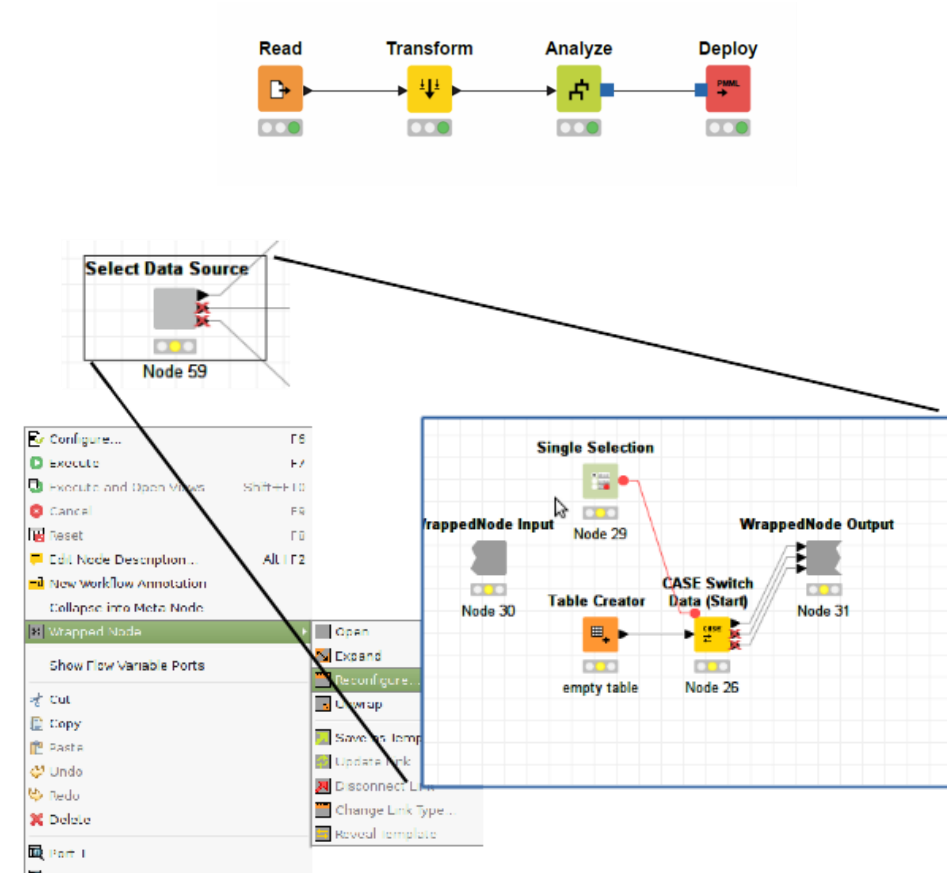
- Simple Regression Tree, Random Forest, Active Learning, ARIMA, k-Means, Prediction Fusion, Rank (New Nodes)
- More In-Database processing nodes

- **Streaming: Executor, Text Processing Nodes**

- **KNIME Server: REST interface, Cloud Server** (license required)

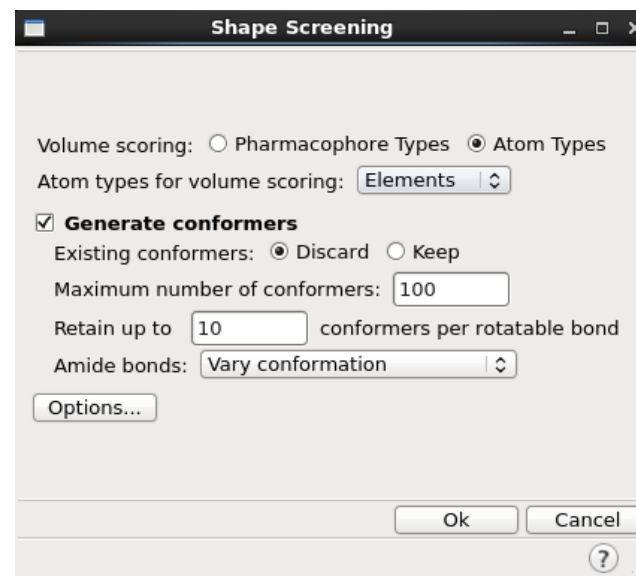
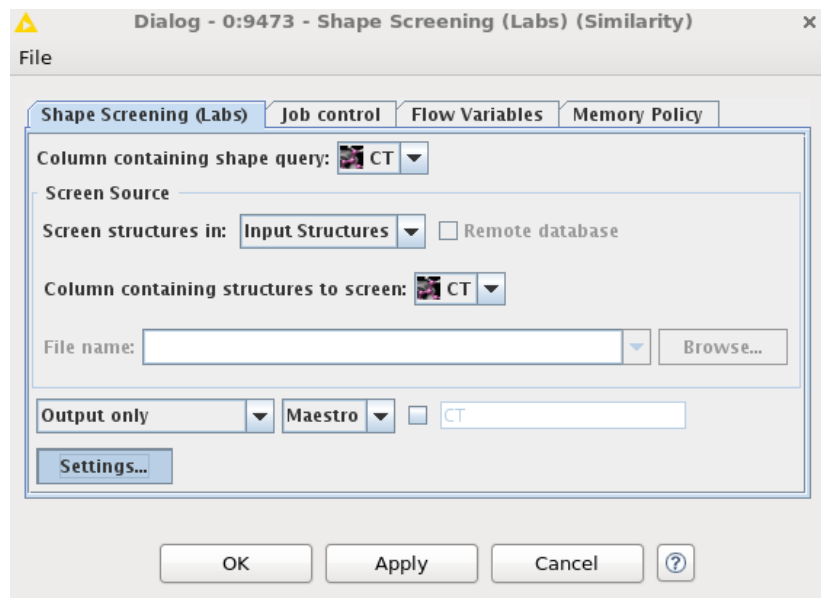
- **KNIME Personal Productivity : WorkflowDiff** (license required)

See details on <https://tech.knime.org/whats-new-in-knime-31> and the full list of changes in the [changelog](#)



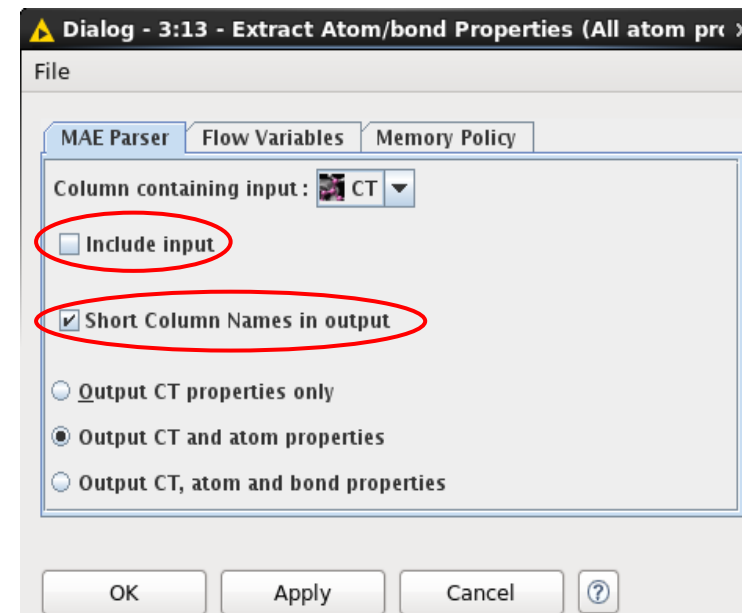
KNIME 3.1 and Shape Screening

- A version compatible with KNIME 3.1 is available for testing:
https://support.schrodinger.com/releases/knime/zipperedUpdateSite/SchrodingerKNIMEUpdateSite_KNIME3.x.zip
 - sdf and mol2 input columns aren't supported yet: a Molecule to Maestro converter node has to be used first.
- New Shape screening node
 - Updated node configuration with the same panel as in Maestro
 - Available in the Labs category and old version still available but deprecated soon
 - URLs supported and editable for an external file to screen (not for a Phase database)
eg knime://LOCAL/... and file:///path/file



Minor Improvements and Fixes

- The parameter flow variables can be used in Strain Rescore node and more Canvas nodes: Generate Pairwise Matrix, Generate Pairwise Matrix (2 inputs), Similarity Matrix
- Short property names and Include input available in the Extract Atom/bond Properties node
- Reader nodes support spaces in the path
- Run Maestro Command supports sdf input
- Ligand size and diameter fields no longer ignored in the Glide Grid Generation node



New and Improved Workflow Examples

- **Shape screening**
 - Pharmacophore – Shape screening: new node
- **Parameter flow variable support**
 - Labs – Parameter flow variables: Force field control for the Glide ligand docking, Strain rescore, Canvas similarity search (to be run on a remote fingerprint file), Generate pairwise matrix, Similarity matrix nodes.

For the nodes using a Python configuration panel, flow variables can't be used to control the options in the panel. However Parameter flow variables can be used to control the equivalent command line options.

This is applicable for the following nodes: Shape screening (labs), IFD (labs), Residue scanning, Conformer cluster.

- **Extract atom/bond properties**
 - Nodes – Node tools: new feature usage

2015-4 New Features

- Includes the latest version of KNIME (v2.12.0)
- Faster and more robust Extract mae atom/bond properties and Extract Maestro properties nodes
- A configured reader node is added when dragging-and-dropping a Grid, Phase hypothesis file into the workspace
- URLs supported and editable in the Molecule Reader node. The output column name is editable
- The Desmond molecular dynamic and Chemistry external tool nodes accept a trajectory as input
- Size property in the Group MAE node

[KNIME Schrödinger extensions version 3.2]

2015-3 New Features

- Compatible with the latest version of KNIME (v2.12.0)
- Better control on calculation distribution
 - Automatically use the maximum number of processors available on the machine
 - Easily change the machine some nodes in a workflow are run on
- New Rotate all and Protein Structure Alignment node improvement
- A configured Molecule reader node is added when dragging-and-dropping a Fasta or a Smiles file into the workspace
- Zipped update site available in the installation
- OPLS3 available in the configuration panel force field list
- Use the same Maestro session to run commands at several stages of the workflow

[KNIME Schrödinger extensions version 3.1]

KNIME 2.12 – some New Features

It was released too late to be included. It will be in 2015-4.

- Log messages in workflow associated with workflow and nodes
- Analytics
 - Rule Handling
 - Statistics measure as aggregation methods in GroupBy node
 - More Statistics Nodes
- Tool Integration
 - Javascript Integration (new interactive visualization nodes)
 - Extended Python Integration (incl. Python edit variable)
- Utility Nodes
 - CASE Switch (eg taking a flow variable as input)
 - GUI Improvements

- Drag&Dropping nodes from the Node Repository over a node or over a connection
- Hotkeys are now available in the Context menu

- KNIME Server & Automation

- REST interface
- Call Local / Remote Workflows from within another workflow
- KNIME Local Automation (New product)

See details <https://tech.knime.org/whats-new-in-knime-212> where you can also find the full list of changes.

KNIME 2.12 – some New Features

Dialog - 0:1208 - GroupBy

File

SettingsDescriptionFlow VariablesJob Manager SelectionMemory Policy

GroupsManual AggregationPattern Based AggregationType Based Aggregation

Aggregation settings

Available columns

MaritalStatus

EstimatedYearlyIncome

NumberOfContracts

Age

Target

Available401K

CustomerValueSegment

ChurnScore

CallActivity

SentimentRating

Products

WebActivity

Select

To change multiple columns use right mouse click for context menu.

Column

Age

Aggregation (click to change)

Missing

Parameter

P^2 Percentile

Edit

add >>

add all >>

<< remove

<< remove all

Scatter Plot

Scatter Plot Test

Investigating new options

Age

SentimentRating

Chart Title: Scatter Plot Test

Chart Subtitle: Investigating

X Column: SentimentRating

X Axis Label:

Y Column: Age

Y Axis Label:

Reset Zoom

Dialog - 2:1206 - Rule Engine (Dictionary)

File

SettingsPMMLFlow VariablesJob Manager SelectionMemory Policy

Rules column: antecedent => consequent

Append column

Prediction

Replace column

WebActivity

Errors

line

rule

error message

Row0

\$gender\$ = "M" => / "Male"/

Not a column: gender

Apply

Use as new default

Close

Workflow Diagram

File Reader

Read iris.csv

Color Manager

Assign colors

Statistics

Calculates statistic measures: mean, max, min, variance, median, etc.

Partitioning

Split data 60/40

Decision Tree Learner

Train model

Interactive Table

Explore test data

Preferences

type filter text

Ant

Data Management

General

Help

Install/Update

Java

KNIME

Chemistry

Databases

KNIME Explorer

KNIME GUI

KNIME Store

Master Key

KNIME

Log File Log Level

DEBUG

INFO

WARN

ERROR

Enable per workflow logs

Log global messages also to workflow log

Maximum working threads for all nodes

Directory for temporary files (you should restart KNIME after changing this)

Improve KNIME

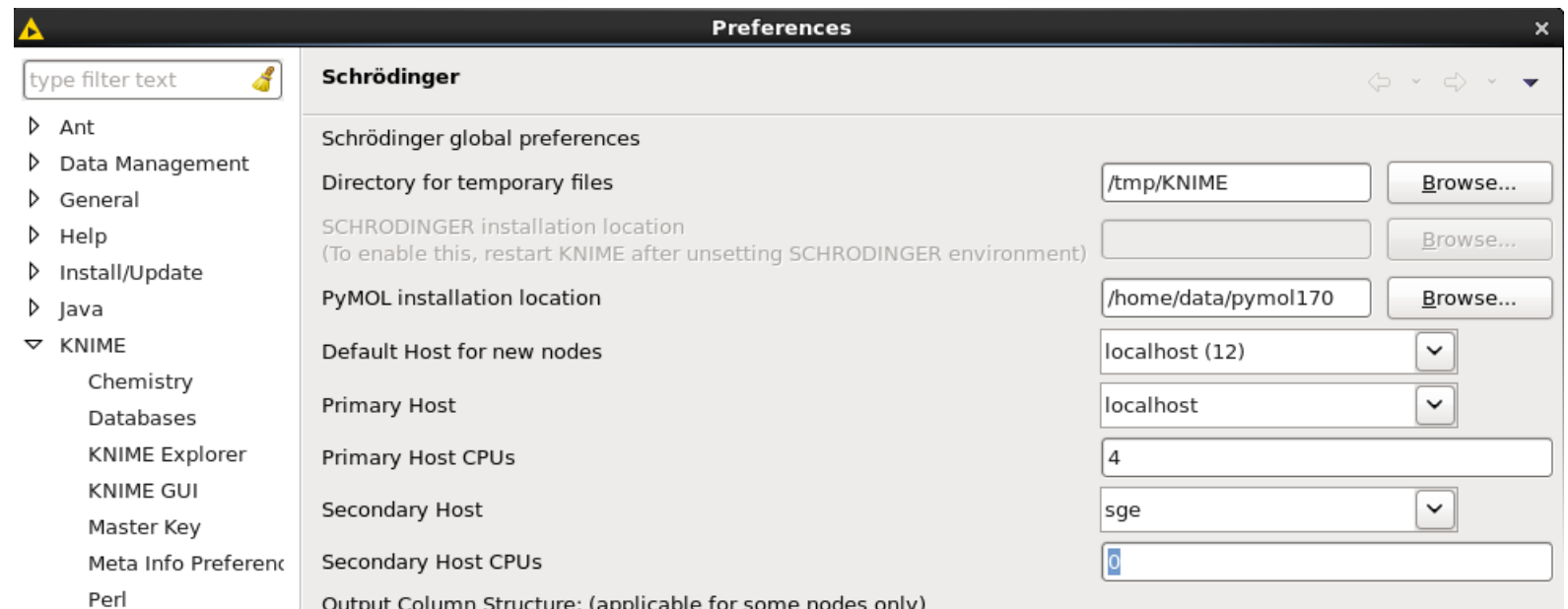
Help us improve KNIME by sending anonymous

Click [here](#) to find out what is being transmitted

Yes, help improve KNIME.

Better Control on Calculation Distribution – Preferences

- Primary and secondary hosts
 - Define PRIMARY_HOST and SECONDARY_HOST placeholders to be used in the Jobcontrol tabs
 - Set the maximum number of processors to be used when the number of processors is set to 0 in the node Jobcontrol tab. If set to 0 in the Preferences all the processors on this machine will be used.
- Default host for new nodes
 - The list includes PRIMARY_HOST and SECONDARY_HOST placeholders



Jobcontrol Panel settings

- #CPUs
 - If set to 0 the node uses the maximum number of processors on the host or set in the Preferences
New default for the new nodes. Use the Primary host as Default host for new nodes to mimic the old behaviour.
- Hostname list
 - Includes the PRIMARY_HOST and SECONDARY_HOST placeholders set in the Preferences
- Separate jobs into subjobs:
 - If turned off it uses the same number of subjobs as the number of processors

Jobcontrol Panel settings

Job control | Flow Variables | Memory Policy

☒ Separate job into: 4 subjobs

Exclude

Column(s): Search

☐ Highlight all search hits

| Hostname | Available # proces... |
|----------------|-----------------------|
| SECONDARY_HOST | 0 |
| fake_local | 3 |
| pdx_web_server | 3 |
| robin_short | 3 |
| centOS32 | 2 |
| sge | 6 |
| localhost | 12 |

Select

Set to Default

add >>

add all >>

<< remove

<< remove all

Include

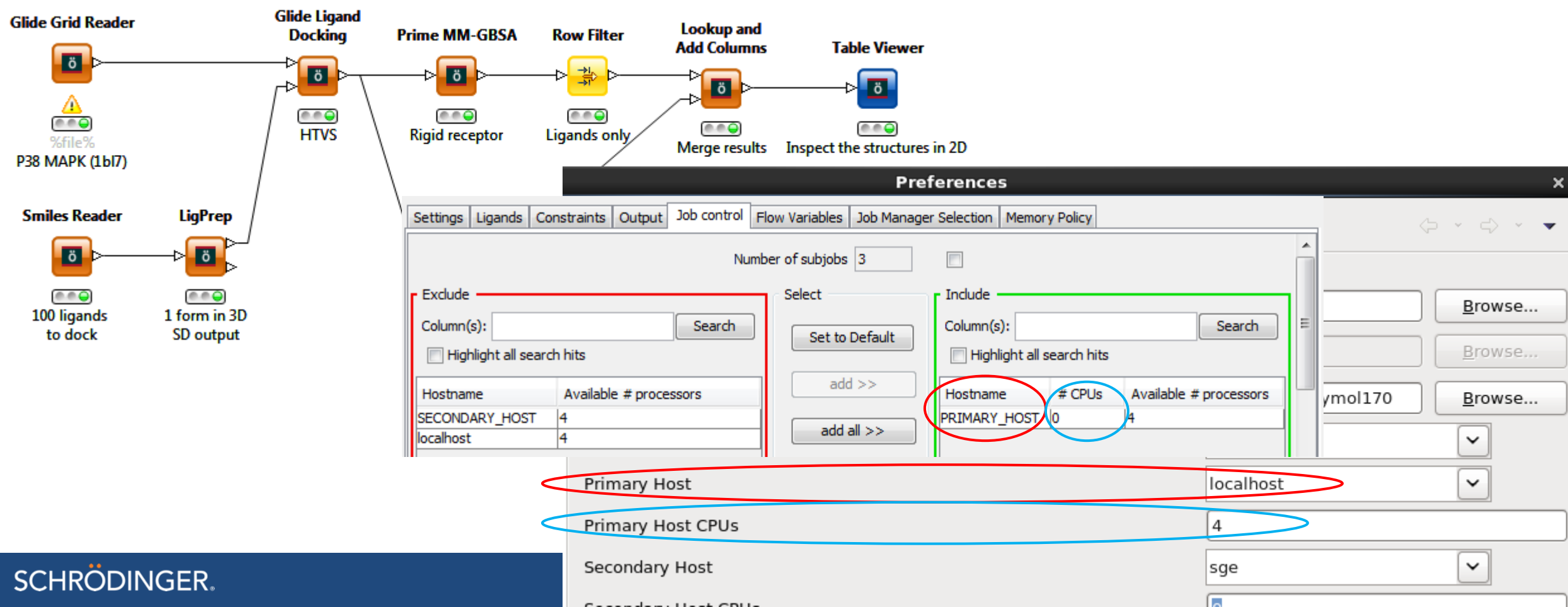
Column(s): Search

☐ Highlight all search hits

| Hostname | # CPUs | Available # proces... |
|----------|--------|-----------------------|
| PRIMARY | 0 | 0 |

Start-up script options

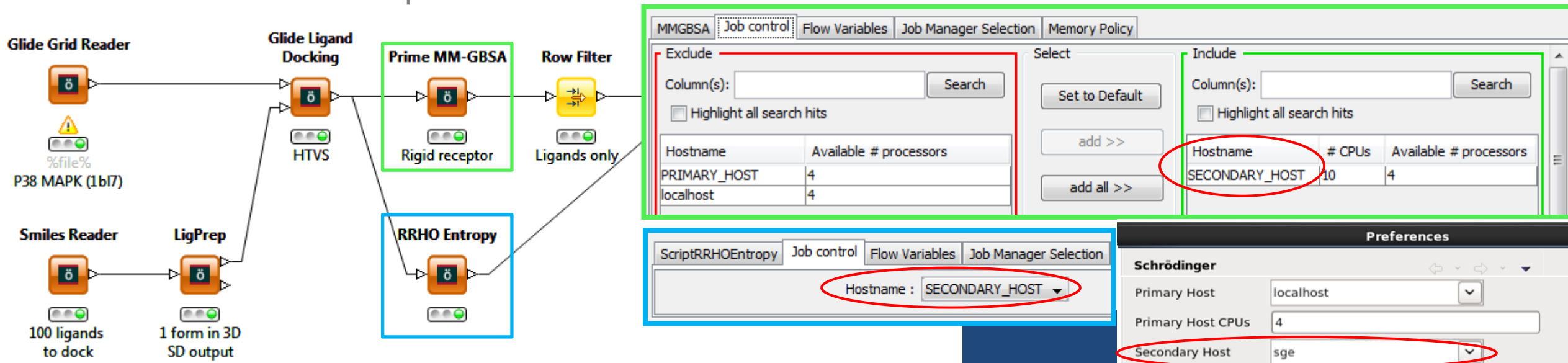
- Corresponding start-up script options
 - –primaryHost (default is localhost), –primaryCPU (default is 0), –secHost and –secCPU
 - The Preferences stored in the workspace are overridden by these options



Better Control on Calculation Distribution – Use cases

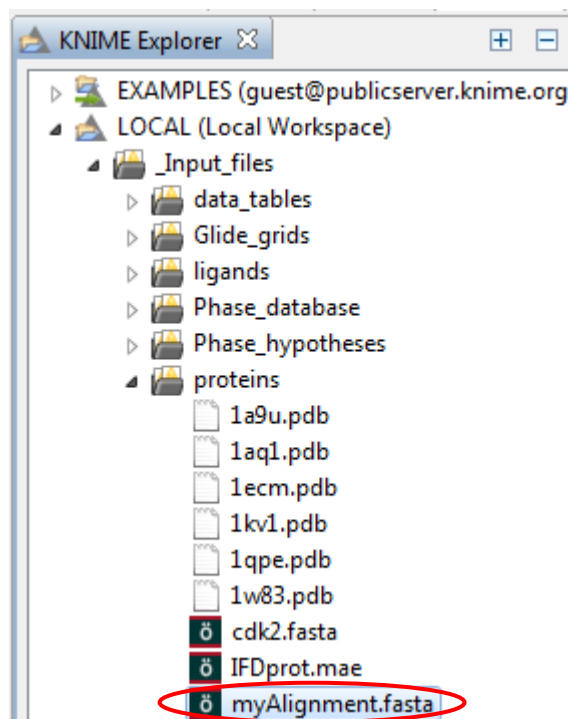
- Workflow to be used on different machines or shared with colleagues
 - Nodes set to use localhost and 0 as number of processors

The host and the maximum number of CPUs specified in the KNIME workspace the workflow has been imported in are used: e.g. my cluster – 12 processors or localhost – 4 processors
- Test a workflow locally before running it on a cluster
 - To test the workflow set computationally expensive calculation nodes to run on the Primary host and 0 as #CPUs in the Jobcontrol tab.
 - In the Preferences set the Primary host to localhost and 2 processors for instance.
 - To run the workflow on a large data set, in the Preferences, change the Primary host to a cluster and 10 processors

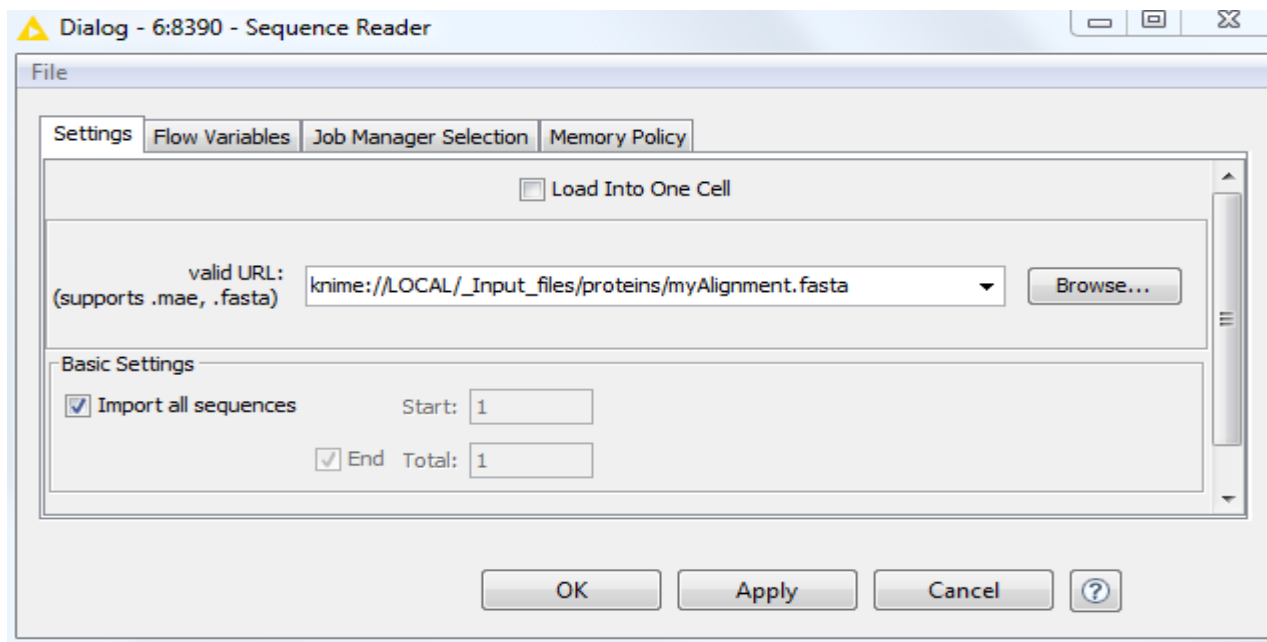


Reader Nodes from a Dragged Smiles or Fasta File

- A Sequence node is added and automatically configured when dragging and dropping a fasta from a file explorer or the KNIME explorer view into the workspace. A Smiles reader node is added for Smiles files.
- This has already been possible for Maestro files associated with the Molecular reader
- Text (.csv and .txt), Mol2 and sdf files are associated with the KNIME Analytics platform reader nodes

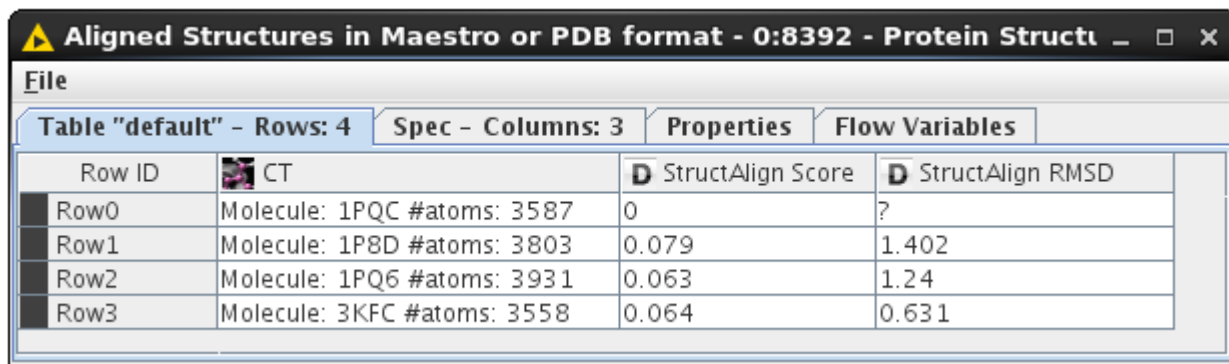


Sequence Reader



Rotate All and Protein Structure Alignment Nodes

- They both align protein structures as rigid bodies, making use of secondary structure information. The Rotate all node initially aligns the first mobile protein and apply the transformation to the remaining mobile structures.
- The alignment score and RMSD are reported and can be used for filtering

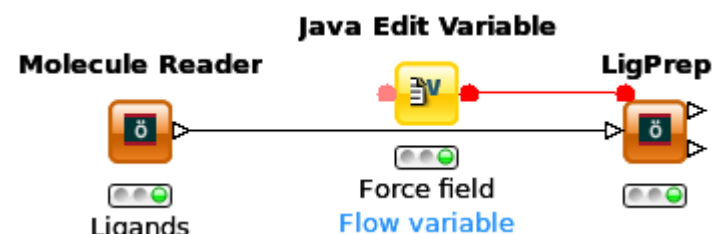
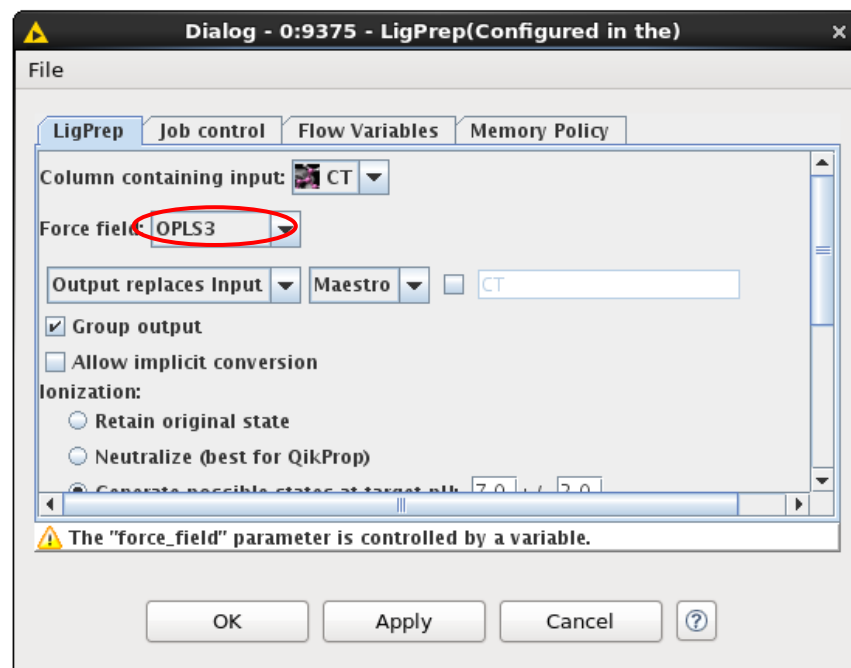


The screenshot shows a software window titled "Aligned Structures in Maestro or PDB format - 0:8392 - Protein Structu". Inside the window, there is a table with the following data:

| Table "default" - Rows: 4 | | | |
|---------------------------|-----------------------------|-------------------|------------------|
| Spec - Columns: 3 | | Properties | Flow Variables |
| Row ID | CT | StructAlign Score | StructAlign RMSD |
| Row0 | Molecule: 1PQC #atoms: 3587 | 0 | ? |
| Row1 | Molecule: 1P8D #atoms: 3803 | 0.079 | 1.402 |
| Row2 | Molecule: 1PQ6 #atoms: 3931 | 0.063 | 1.24 |
| Row3 | Molecule: 3KFC #atoms: 3558 | 0.064 | 0.631 |

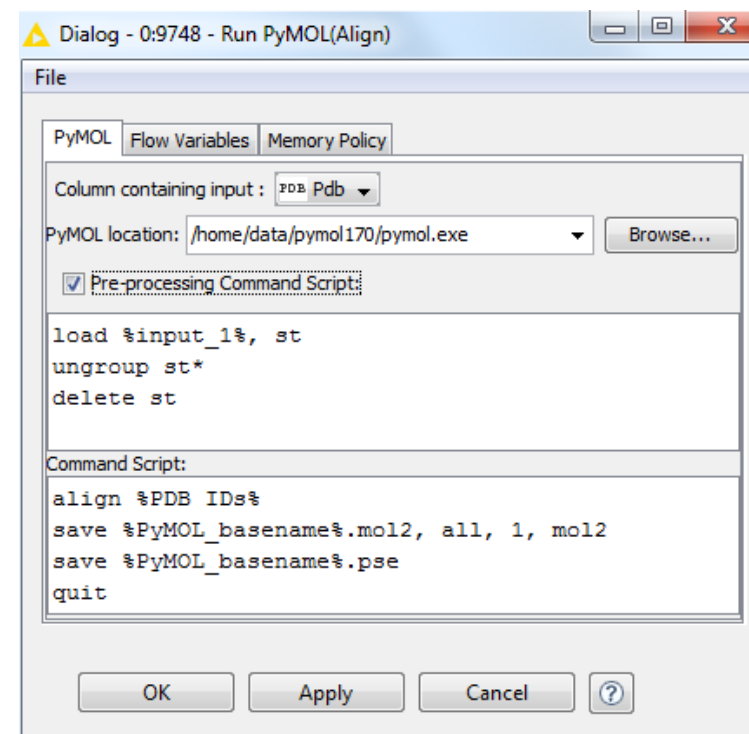
OPLS3 in the Force Field List

- The force field can be set to OPLS3 in the configuration panel force field drop down list
- Reminder: the configuration panel options can be controlled by simple flow variables and don't require Parameter flow variables



Minor Improvements and Fixes

- Use the same Maestro session to run commands at several stages of the workflow
 - Using `pythonrunbuiltin KNIME_maestro_connector.send` command in the KNIME-Maestro connector node
- Zipped update site available in the installation:
 - `$SCHRODINGER/knime-v*/data/SchrodingerKNIMEUpdateSite_3.1.7.201506160750.zip`
 - Easy access to add the extensions to or update a stand-alone installation`KNIME_install.py` could also help installing a set of extensions (not only Schrodinger ones)
- The Shape screening node runs the new fast algorithm.
The old method can still be used with a the Parameter flow variable `ShapeScreen-classic`
- Better logging in Protein Preparation Wizard
- Molecule-To-MAE node reports the exit status of the converter
- Preprocessing command script section added to Run PyMOL



New and Improved Workflow Examples

- **Better control on calculation distribution**
 - All workflow examples are set to run on the Primary host and the number of CPUs specified in the Preferences. So these can easily be changed to run on your machine of choice and number of CPUs.
 - Docking - Docking: illustrates all the new functionality
- **Rotate and Protein Structure Alignment**
 - Protein- alignment workflow example
- **Smiles and Fasta readers**
 - Used in Protein - Model building and Cheminformatics - Clustering workflows for instances.
- **OPLS3**
 - Lab - Parameter flow variable use-cases: the force field can be set to OPLS3 using a simple flow variable
- **Use again the same Maestro session to run commands**
 - General - Run Maestro command use cases: so Maestro window can be put in the background
- **Phase Shape**
 - Lab - parameter flow variable use-cases: to use the old algorithm

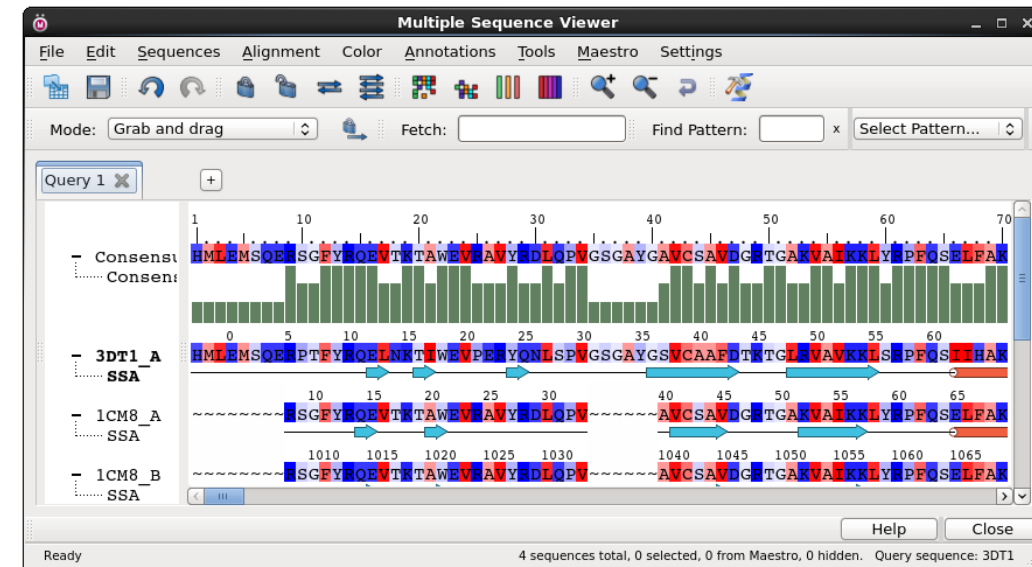
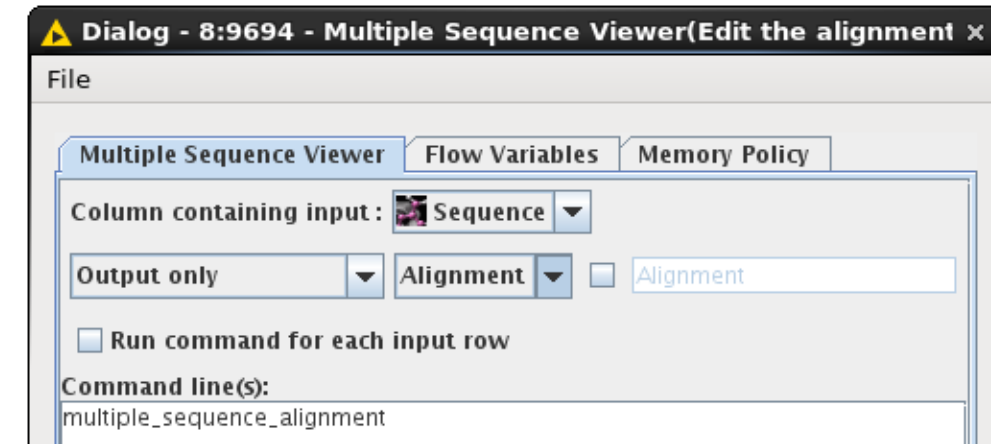
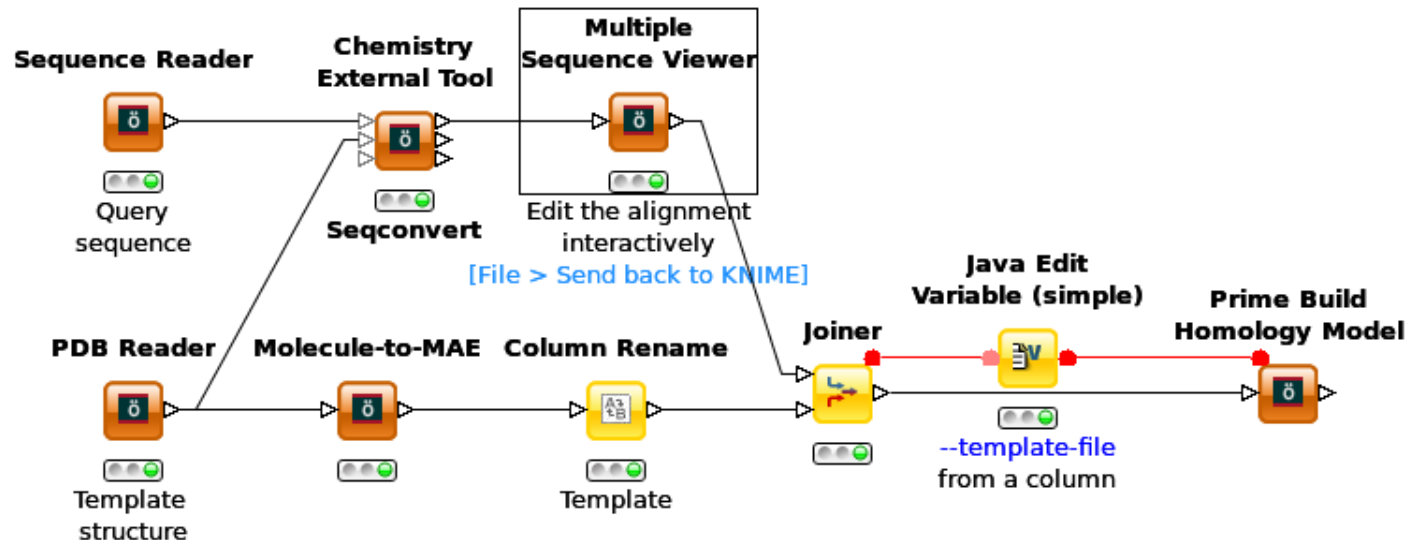
2015-2 New Features

- Includes the latest version of KNIME (v2.11.3)
- New **Multiple Sequence Viewer** node
- Molecule reader node URL editable to use “knime:” and “file:”
- The **parameter flow variables** can be used in LigPrep, Molecule reader and Molecule-to-MAE nodes
- Easy way to list the command line options to be used as Parameter flow variables
- **Free nodes** don't require a Schrödinger installation when possible
- Residue scanning and Conformer cluster configuration panel start-up faster
- Run Maestro command and Jaguar minimization nodes are more robust

[KNIME Schrödinger extensions version 3.0]

Multiple Sequence Viewer

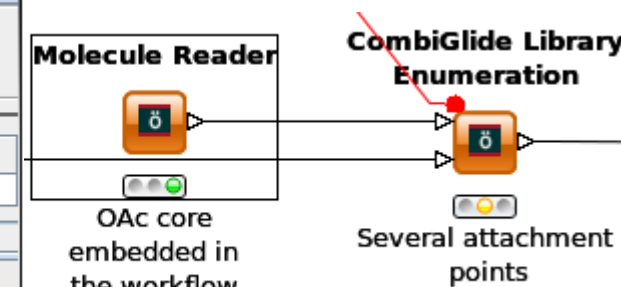
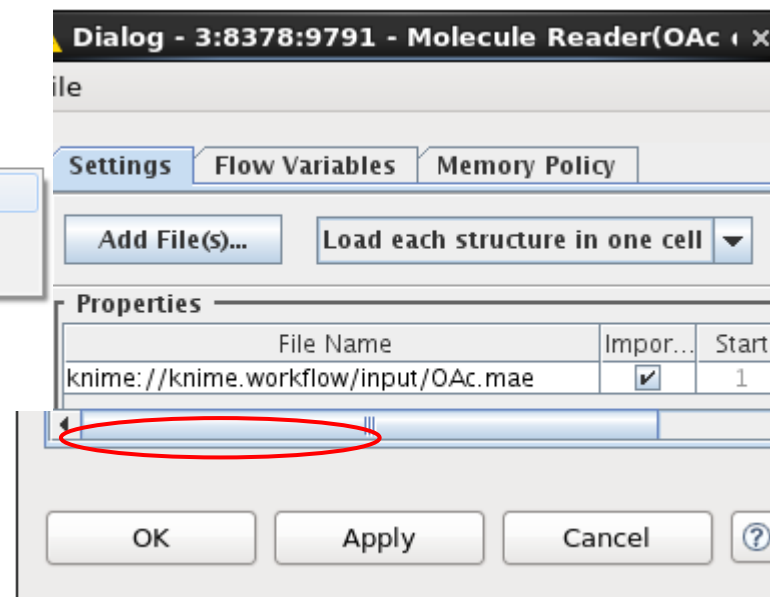
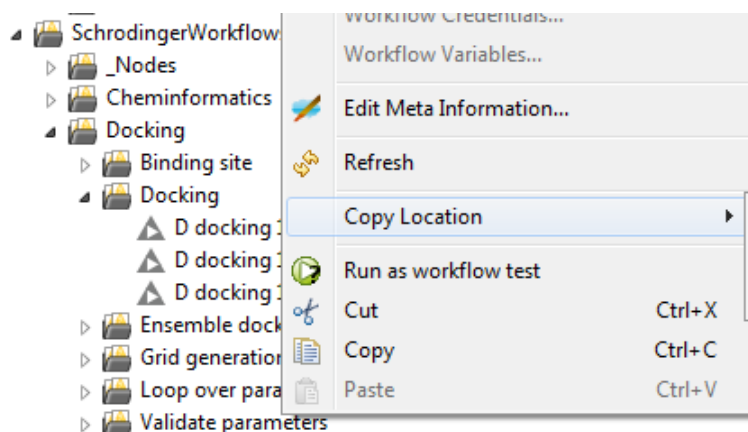
- Sequence and alignment visualization and manipulation
- Command section
 - Allows for automation of some tasks
 - See the list of the commands in the node description including `send_to_knime` for headless use of the MSV



Molecule Reader Editable URL

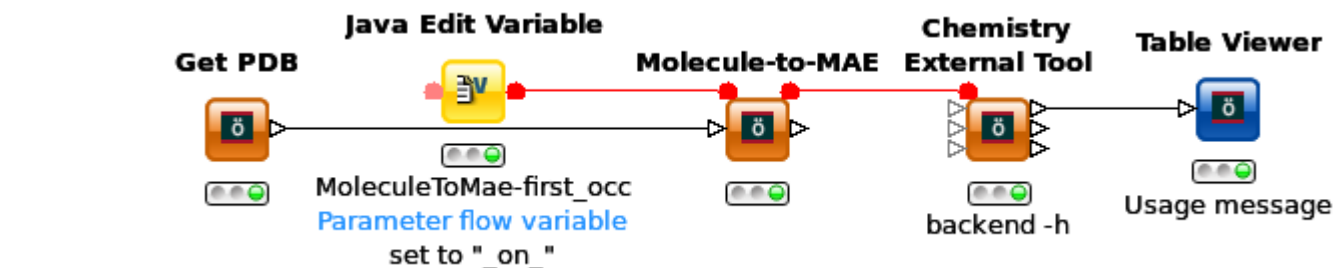
Molecule reader node URL is editable so as to point to:

- A file embedded in the workflow
 - `knime://knime.workflow/<directory in the workspace workflow folder>/<filename>`
 - Usage: embed input files
 - Get the path of the workflow folder from the pop-up menu in the KNIME explorer > Copy Location
- A file in the workspace
 - `knime://LOCAL/<workflow group(s)>/<filename>`
 - Similar to dragging and dropping a file stored in the workspace
- A file on disk
 - `file:/<path on disk>/<filename>`
 - Similar to dragging and dropping a file from a file explorer in the workflow
- First configuration with a (possibly mock-up) file



Parameter Flow Variables and Option List

- The parameter flow variables can be also used in LigPrep, Molecule reader and Molecule-to-MAE nodes
- Easy way to list the command line options that can be used as Parameter flow variables:
 - Use the backend flow variable available in these nodes



Molecules in Maestro format - 1:9382 - Molecule-to-MAE

| File | | | | |
|---------------------------|----------|-------------------------|--|----------------|
| Table "default" - Rows: 1 | | Spec - Column: 1 | Properties | Flow Variables |
| Index | Owner ID | Name | Value | |
| 0 | 1:9382 | backend | /home/data/schro-NB/utilities/pdbconvert | |
| 0 | 1:9382 | MoleculeToMae-all_occ | | |
| 0 | 1:9382 | MoleculeToMae-first_occ | | |

Command line(s):
`%backend% -h 1 > %output_1% 2 >> %output_1%`

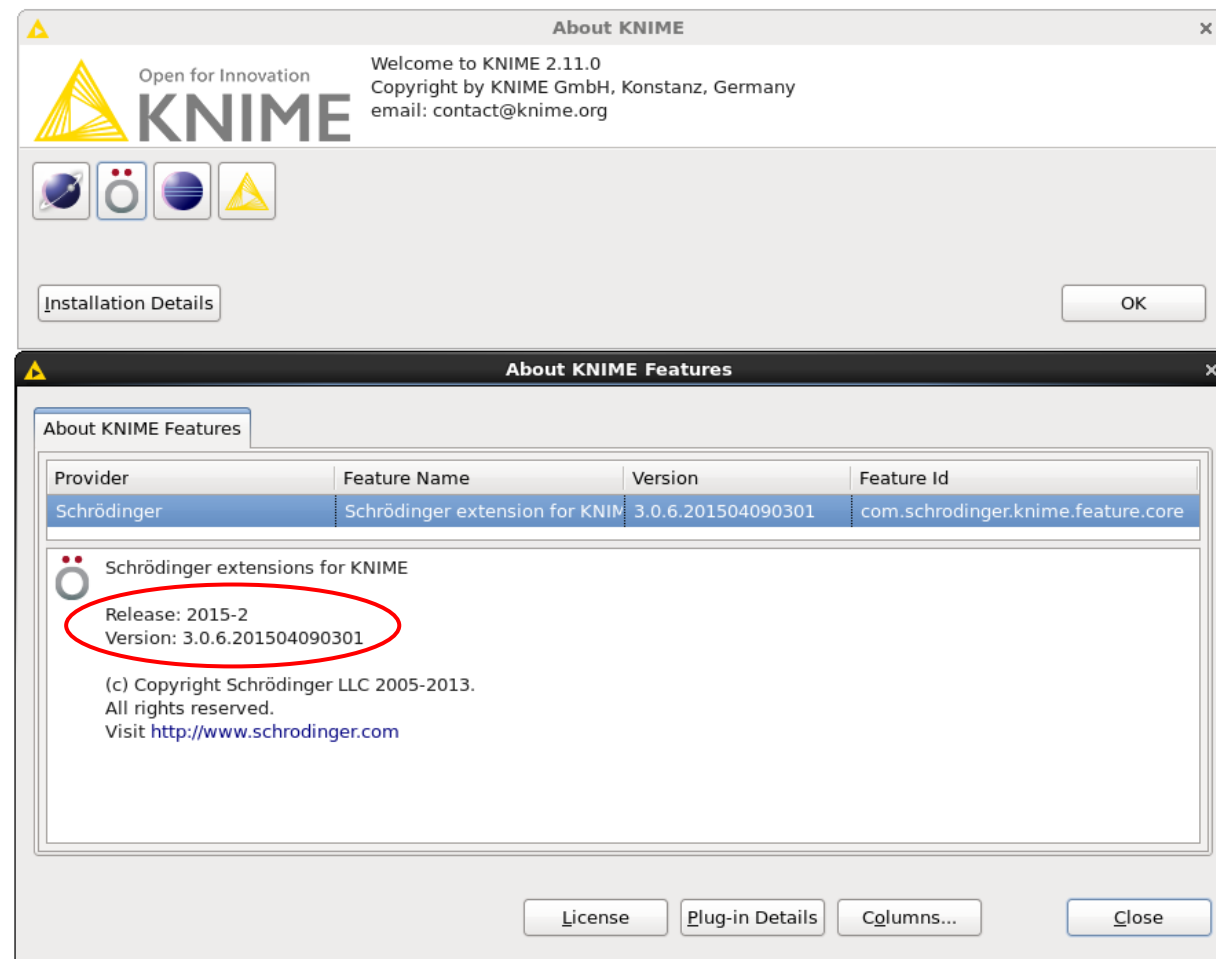
Row: Row0 Column: Usage Type: TextFileCell

| File | Usage |
|---------------------|--|
| -ignore_obsolete | : Don't exit on seeing OBSOLETE record in a pdb file |
| -warn_obsolete | : Warn on seeing OBSOLETE record in a pdb file |
| -histidine <mode> | : HIS protonation mode when residue lacks hydrogens protonation <mode> is one of: delta : only ND1; neutral residue (default) epsilon : only NE2; neutral residue protonated : both ND1 and NE2; +1 total res charge |
| -occ <sites> | : For atoms with alternate sites with different occupation factors, specify which to read. <sites> is one of: all : read all alternate sites (default) first : read first occ site listed per atom |
| -first_occ | : equivalent to -occ first |
| -all_occ | : equivalent to -occ all |
| -charge <mode> | : Termini protonation <mode>, one of: ph7_protonate_caps : protonate termini, identified from SEQRES records if available (default) full : protonate chain breaks as well neutral : do not add formal charges |
| -use_component_dict | : use residue information from component dictionary |
| -no_component_dict | : don't use residue information from component dictionary (default) |
| -noindex | : On pdb->mae conversion don't update the indexing properties to store the index of file on conversion. By default it stores source file and structure index. |

Minor Improvements and Fixes

- Residue scanning and Conformer cluster configuration panel start-up faster
- Run Maestro command and Jaguar minimization nodes are more robust
- Plugin version number changed to: mmshare version – date

See Help, About KNIME, Schrödinger icon



Some Free Nodes don't Require a Schrödinger Installation

They don't require any Schrödinger installation when possible and otherwise only a Maestro installation

- **Reader, Writer** and Converter nodes
- Visualization: **Run PyMOL, Run Maestro, KNIME-Maestro connector, Multiple sequence viewer**, Run Spreadsheet viewer, Table viewer
- Scripting: **Chemistry external tool node**, Run Maestro command
- Tools: **Workflow List**, Setup Diagnosis nodes
- Utility script: KNIME_install.py

See details in:

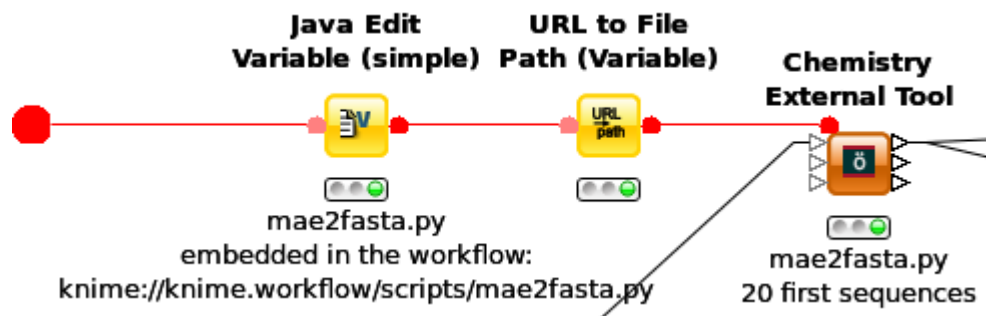
https://www.schrodinger.com/knimeworkflows/KNIME_Free_Nodes.pdf

Requirement and Setup

- For the Workflow List, Run Spreadsheet viewer, Table viewer, Chemistry external tool nodes:
 - Install Schrödinger **free nodes**:
<https://www.schrodinger.com/SchrodingerKNIMEFreeNodes>
<http://tech.knime.org/community> - update site: <http://tech.knime.org/update/community-contributions/2.11/>
On Windows the Chemistry external tool and Workflow list nodes require specific set-up (see [KB#1925](#))
- For the Run PyMOL node:
 - In Workspace Preferences, point to any PyMOL installation
- For all the other free nodes and the utility scripts:
 - In Workspace Preferences, point to a Maestro installation
Maestro is free of charge for all academic users and commercial users who purchased one of the Schrödinger tools
Installer and license from <https://www.schrodinger.com/freemaestro/> (also includes the zipped update site)
 - The install script is available from https://www.schrodinger.com/KNIME_install/KNIME_install.zip

New and Improved Workflow Examples

- **Multiple Sequence Viewer**
 - Nodes – MSV: simple example
 - Protein – Model building and Real world examples – Protein model building: new node use cases
- **Parameter flow variables**
 - Lab – Parameter flow variables: illustrates more node use cases. Based on the backend flow variable the command line options that can be used are listed.
- **Molecule reader node accepts “knime:” and “file:” URLs**
 - Nodes – Readers and Writers: simple example
 - Pharmacophore – Shape screening and many other workflow examples: point to input files stored in the workspace
 - Protein – Model building: same URL format used to use a script embedded in the workflow

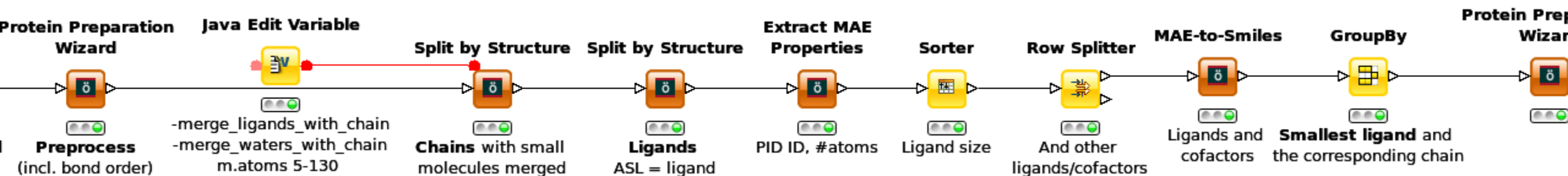


New and Improved Workflow Examples

- KNIME UGM workflow

- Real world example – Cocrystallized ligand redocking: improved ligand detection process

Derived from the work published by Paulette Greenidge from Novartis in: J. Chem. Inf. Model. 2014, 54(10), 2697–717



- Free nodes

- Nodes – Free nodes: specific examples using only free nodes.

- Simple workflow examples

- Nodes – Reader and writer nodes: including reading a list of PDB files in a folder
 - Nodes – Run Maestro and Run Maestro commands
 - Nodes – Workbench: list of the most commonly used nodes

2015-1 New Features

- Includes the latest version of KNIME (v2.11.0)
- **KNIME-Maestro Connector** improvements to replace the **Run Maestro 1:1** metanode
- New **Conformer cluster** node
- Run the Workflow list node on a selected workflow group
- The simplified batch execution script KNIME_batch.py must now be run without -FROM maestro
- The Schrödinger extensions in a stand-alone KNIME installation only requires setting \$SCHRODINGER environment variable
- Simplified KNIME_install.py invocation to install all community nodes
- A specific executable file can now be chosen in the Run PyMOL node installation field

[KNIME Schrödinger extensions version 2.9]

KNIME 2.11 – some New Features

- Database and Big Data Extension

Database GroupBy improvement, Drop Table, HP Vertica Connector, Impala Connector / Loader, HDFS Connector / File Permissions new nodes

- Tool Integration

- JSON Processing
- New Python Integration

- Data Mining

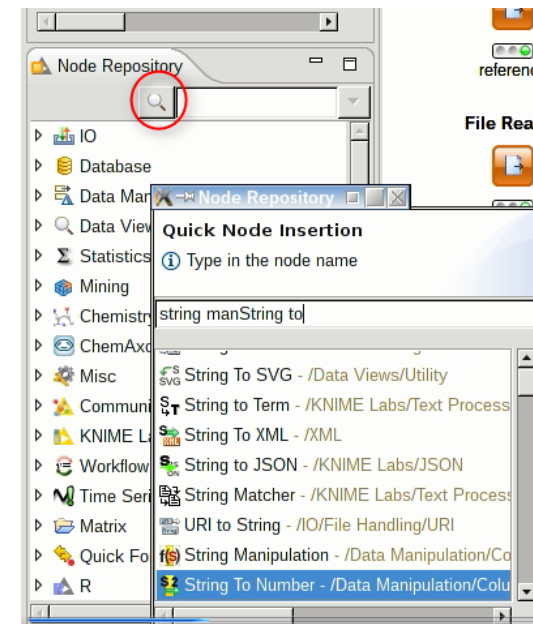
Modular PMML, DBSCAN density based clustering algorithm, kNN now supports more distance functions, Target Shuffling

- IO – Writer Nodes Improvements

- Other

- Quick Node Insertion with Ctrl-Space (New GUI feature)
- Table Validator and Column Auto-Type Cast new nodes

See details in <http://tech.knime.org/whats-new-in-knime-211> and full list of changes in [changelog file](#)



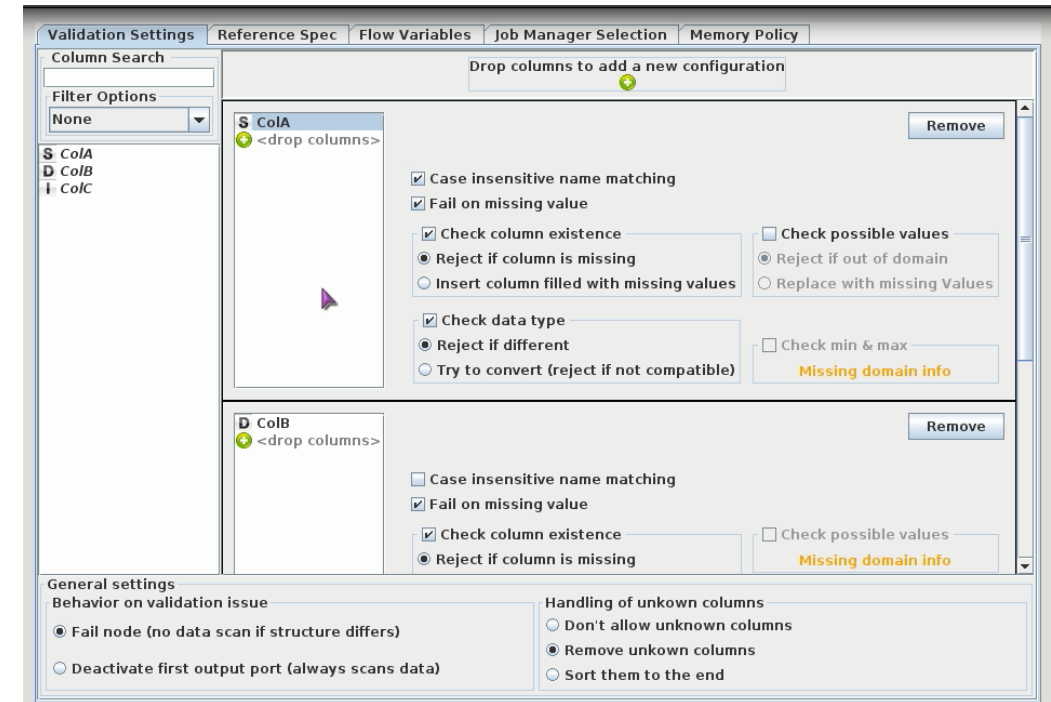
KNIME 2.11 – some New Features

- **New Python Integration**
 - based on CPython
 - Schrödinger Python installation can be used after installing Protobuf (for the communication between CPython and KNIME) and optionally Jedi (for the auto-completion)
- **Column Auto-Type Cast**

tries to guess the most fitting type for a specified column. It is useful after a Transpose and before transforming a data cell into a flow variable.

- **Table Validator**

checks the input table format against missing values, out of domain values...

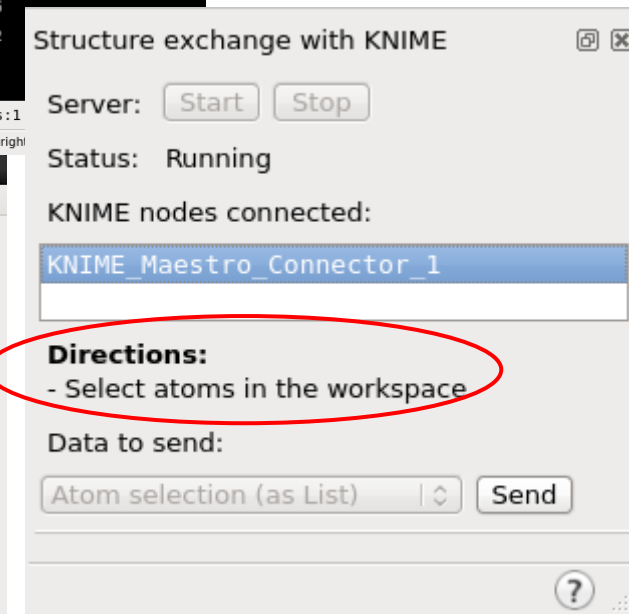
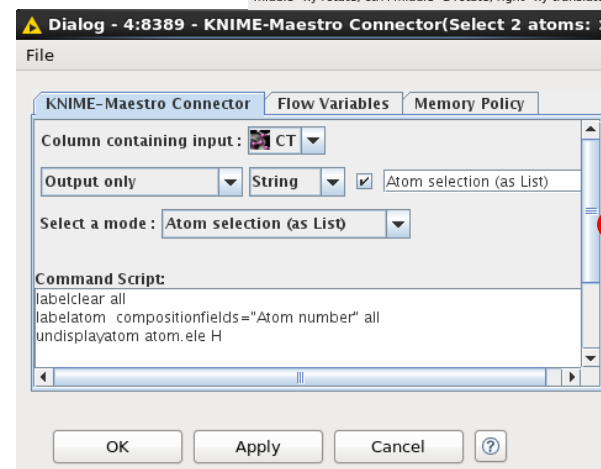
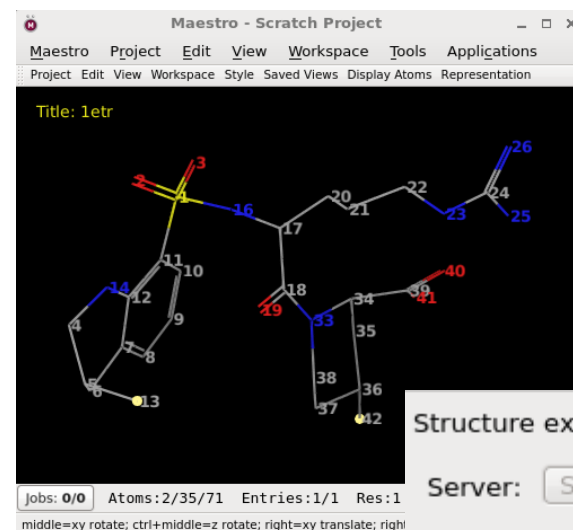


Path, Environment, and Update Simplifications

- Simplified batch execution script KNIME_batch.py must now be run without -FROM maestro:
eg `$SCHRODINGER/run KNIME_batch.py -stdout INFO "D vs 1.zip" -schrodingerTempDir /tmp/KNIME -run -isdf ligands.sdf -igrd fxa_grids_recep -osdf /tmp/out.sdf`
- A stand-alone KNIME installation now only requires setting \$SCHRODINGER
See KB#1696 for other ways to run Schrodinger nodes in a stand alone installation
- Simplified KNIME_install.py script invocation
 - e.g. 1 command line to add all the trusted community nodes (<http://tech.knime.org/community>) to the embedded KNIME installation:
`"$SCHRODINGER/run" -FROM knime KNIME_install.py`
`-features_list "$SCHRODINGER/knime-v*/data/full_free_features.lst" "$SCHRODINGER/knime-v*/bin/*/knime/"`
 - The KNIME version embedded in \$SCHRODINGER/knime-<version>/bin/<os>/knime
 - Is identical to the download from KNIME web site
 - Only some basic extra features are added to keep the size under control but others can easily be added from the GUI or using KNIME_install.py

KNIME-Maestro Connector Improvements

- KNIME-Maestro Connector improvement to replace the Run Maestro 1:1 metanode
- Make some selections/structure changes interactively
- New modes:
 - All entries, Selected entries
 - CombiGlide core definition
 - Atom selection (as List, Names, ASL, SMARTS)
 - Residue selection (as List, ASL)
- Command script section
- Iterate over entry structures
- Dockable panel



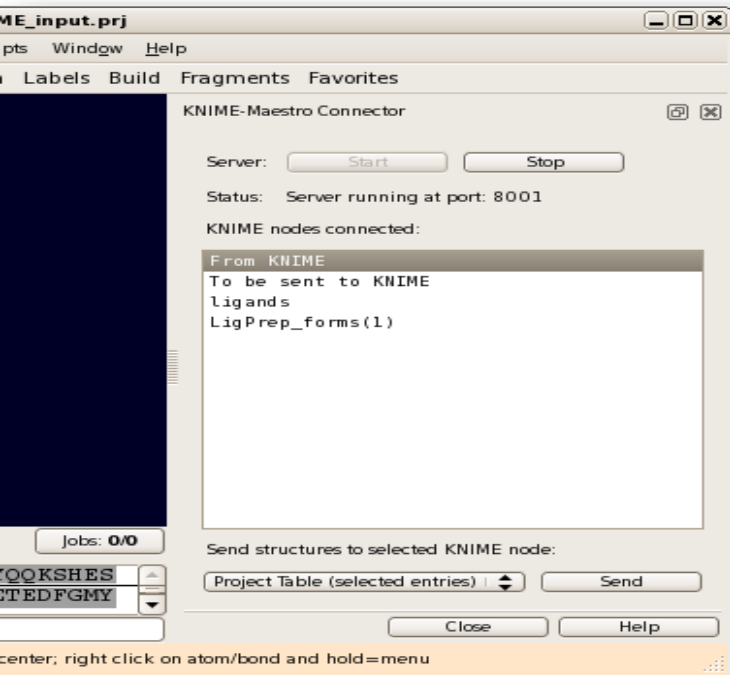
Maestro - KNIME structure exchange (since 2012)

Maestro

Server

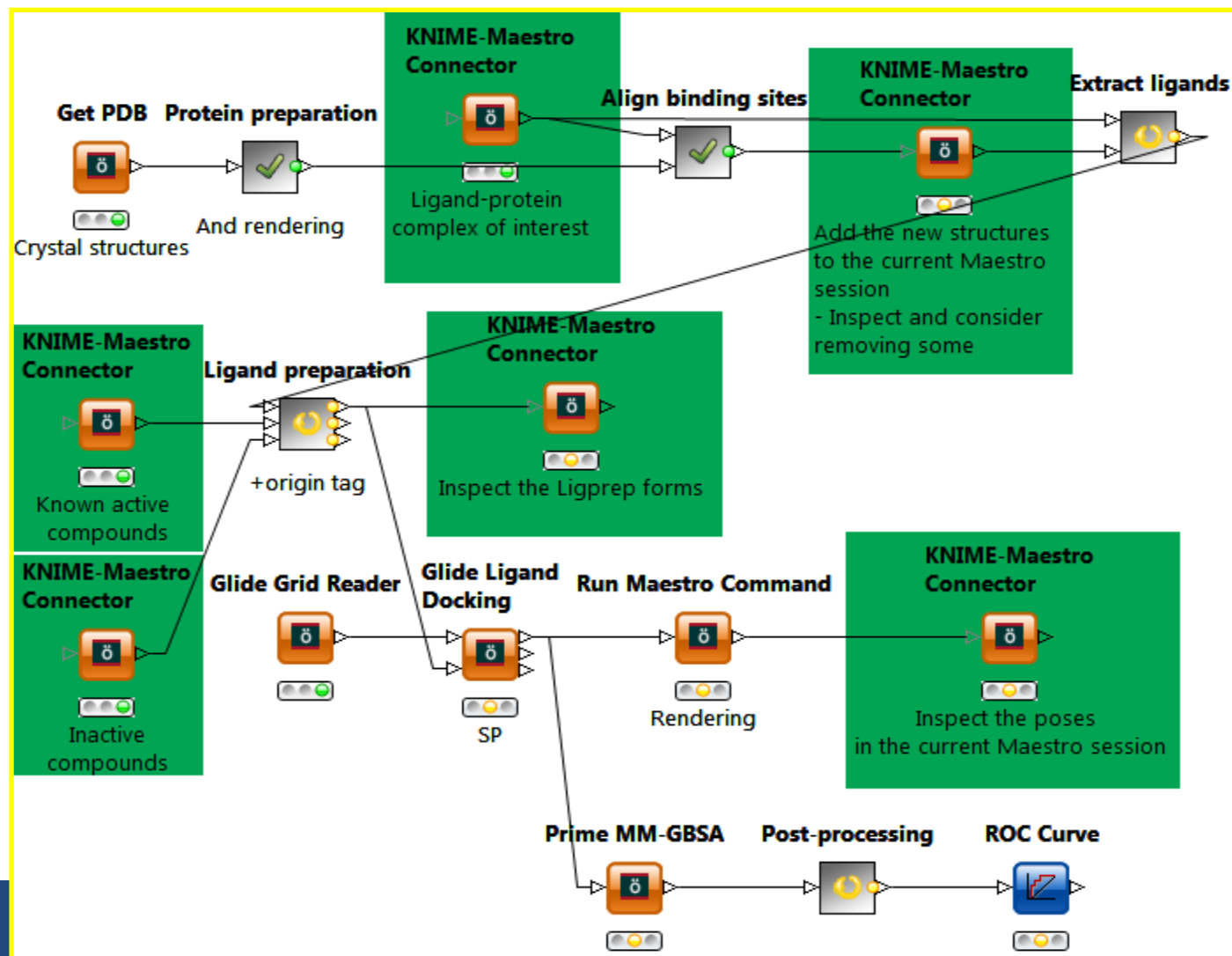
KNIME

<http://www.schrodinger.com/knimeworkflows/>
Validate docking parameters



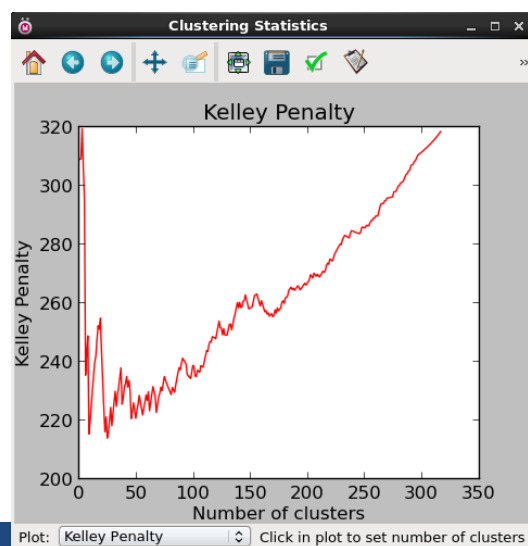
Project table

| Row | Stars | In | Title | docking score |
|------|-------|----|------------------------------------|---------------|
| [3] | | - | [1] - Crystal structures | |
| 1 | ☆☆☆☆ | ☐ | 1AC8 | |
| 2 | ☆☆☆☆ | ☐ | 1AET | |
| 3 | ☆☆☆☆ | ☐ | 1AC4 | |
| [8] | | + | [2] - Known active | |
| [17] | | + | [3] - Inactive compounds | |
| [54] | | + | [4] - Ligprep forms | |
| [55] | | - | [5] - MaestroCmd_34402818517213... | |



New Conformer Cluster Node

- The new Tools > Conformer Cluster node is configured with the same panel as in Maestro
- Interactive or automatic selection of the number of clusters
 - Visually or based on the Kelley penalty
- Same look and feel as the other KNIME nodes
 - Cancel, Reset, Job control distribution ...
 - Parameter flow variables, batch execution



The figure shows the "Conformer Cluster" dialog box. It has a title bar with a logo and standard window controls. The main section is titled "Generate RMSD Matrix" and contains the following options:

- Cluster by:** ☒ Atomic RMSD ☐ Torsional RMSD
- ASL:**
- Buttons:** Heavy Atoms + OH, SH | Heavy Atoms | All Atoms
- ☒ Retain mirror-image conformers
- ☐ Perform structure equivalence test for large molecules
- ☐ Output structure with ☒ More negative ☐ More positive per cluster
- ☐ RMSD in place

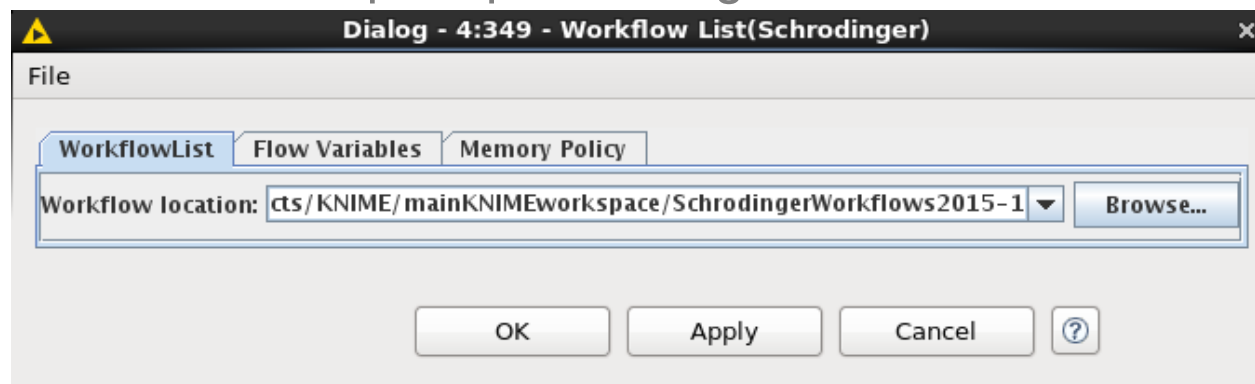
The "Clustering" section has three tabs: "Calculate" (selected), "Results", and "Apply".

- Linkage**
 - Linkage method:
- Cluster**
 - Clustering is performed on the input structures using the RMSD matrix and similarity settings.
 -

At the bottom right are "OK" and "Cancel" buttons.

Minor Improvements

- Run the Workflow list node on a selected workflow group
Faster execution and easier post-processing

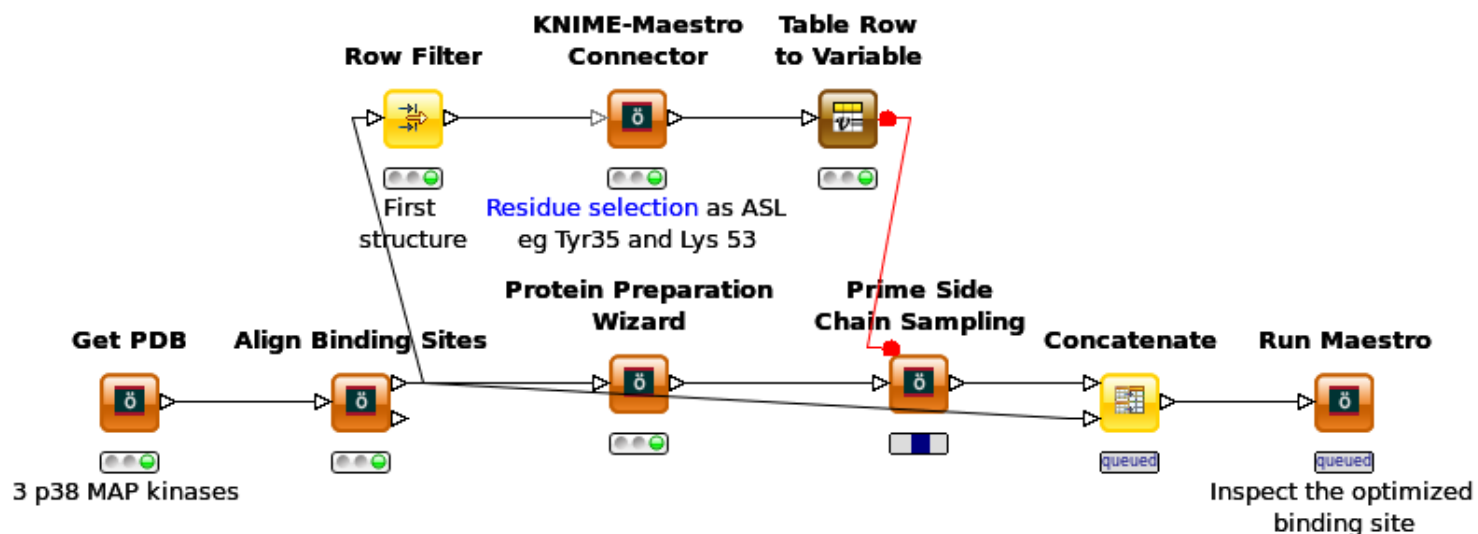


- A specific executable file can be chosen in the Run PyMOL node installation field



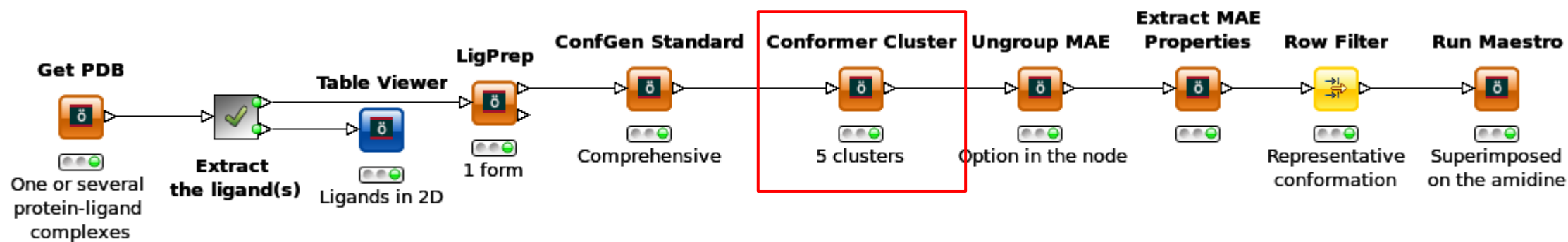
New and Improved Workflow Examples

- KNIME-Maestro connector node replacing the Run Maestro 1:1 metanode in:
 - Labs – Run Maestro 1:1 metanode use-case example moved to General – KNIME-Maestro Connector (residue selection, create more entries)
 - General – Python script, Molecular Mechanics – Conformational search and Molecular Dynamics – Simulation (atom selection for distance measurement)
 - Quantum Mechanics – Conformational search (dihedral angle selection)
 - Library design – Library enumeration (core attachment point selection)
 - See also Docking – Validate parameters – KNIME-Maestro connectors (initial mode: existing Maestro session)



New and Improved Workflow Examples

- Conformer cluster
 - Nodes – Conformer cluster (simple usage examples)
 - Molecular Mechanics – Conformational search (new node application)



work with Paulette Greenidge:

“Improving Docking Results via Re-ranking of Ensembles of Ligand Poses in Multiple X-ray Protein Conformations with MM-GBSA PA Greenidge”, C Kramer, JC Mozziconacci, W Sherman. Journal of chemical information and modeling. 2014, 54 (10), 2697-2717

New and Improved Workflow Examples

- Real world applications – Protein model building
Including a Multiple Sequence viewer metanode and homology model building on a specific template
- Nodes – Epik
Simple usage examples
- General – Installation update/creation
Add the trusted community nodes in one command. Can even be used on the running installation
- General – Batch execution
New workflow illustrating KNIME_batch.py options and execution
- Pharmacophore – Shape Screening and Docking – Virtual screening and General – Run PyMOL and Workflow list
Updated

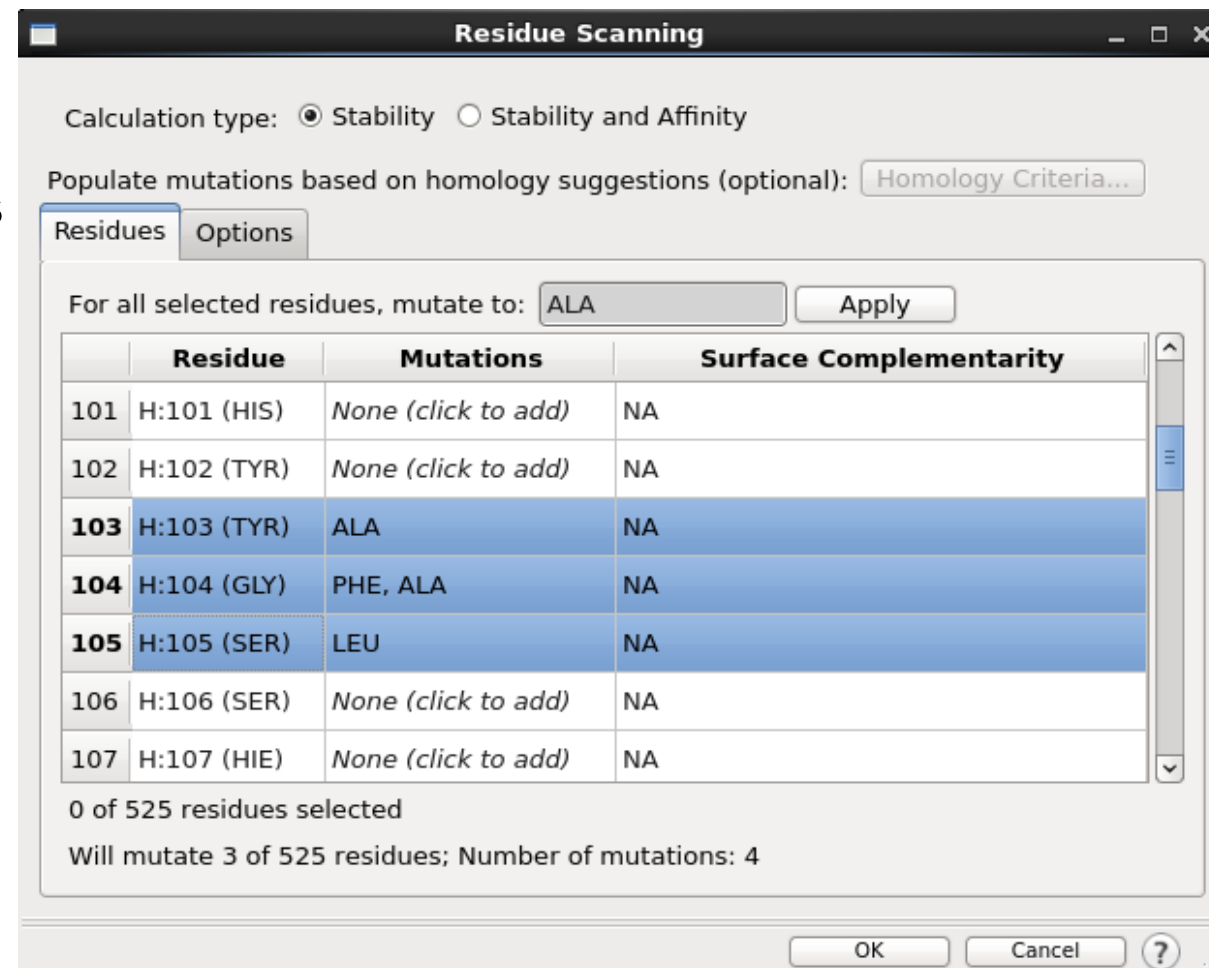
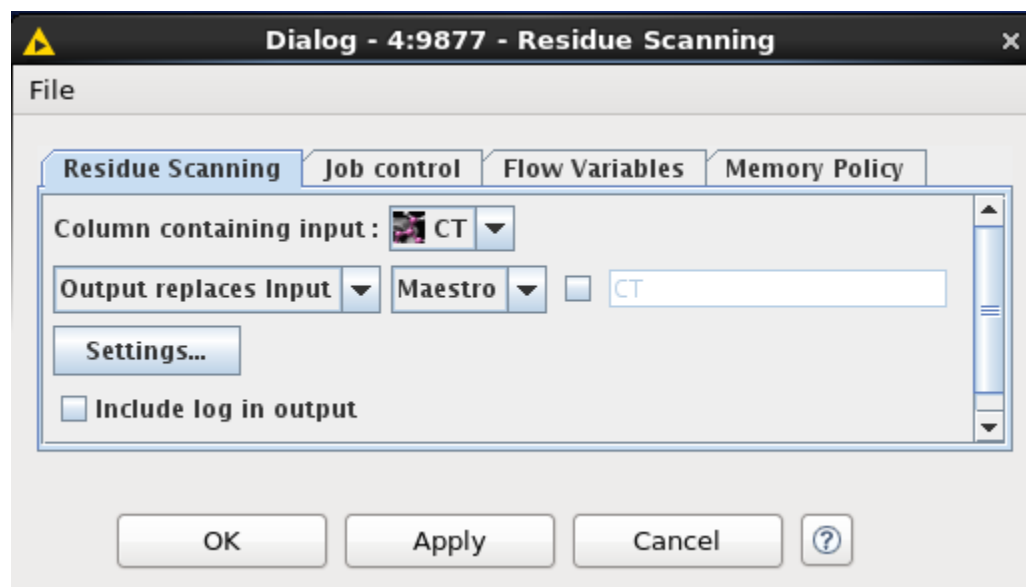
2014-4 New Features

- Includes the latest version of KNIME (v2.10.1)
- New **Residue scanning/affinity maturation** node that uses the same configuration panel as Maestro
- **Run PyMOL output files** can be used by downstream nodes
- **Pop-ups no longer block Run Maestro** and Run Maestro command nodes
- Improved loading of Schrödinger extensions during KNIME start-up

[KNIME Schrödinger extensions version 2.8]

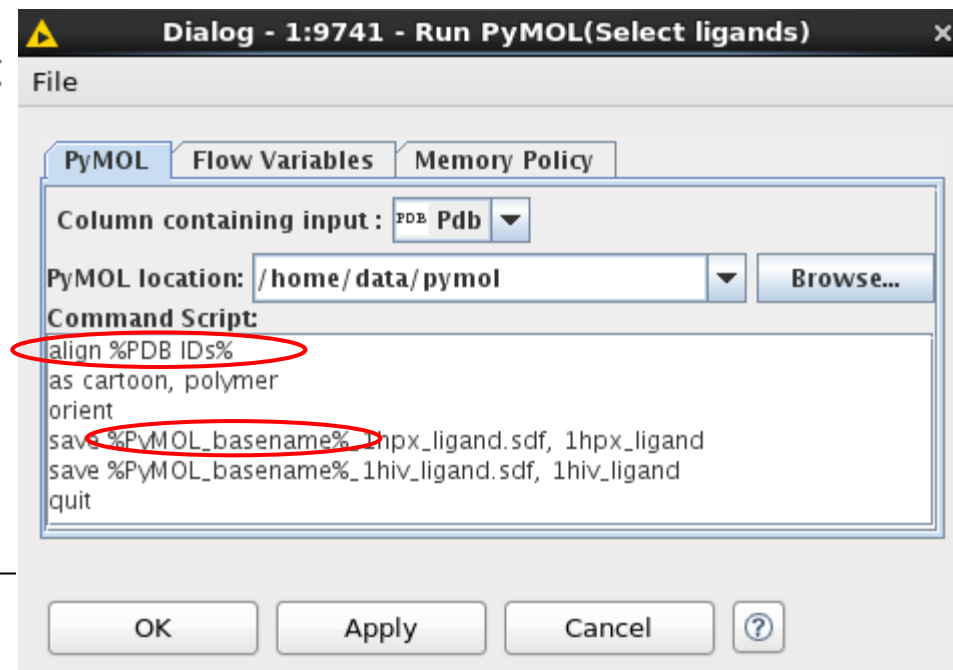
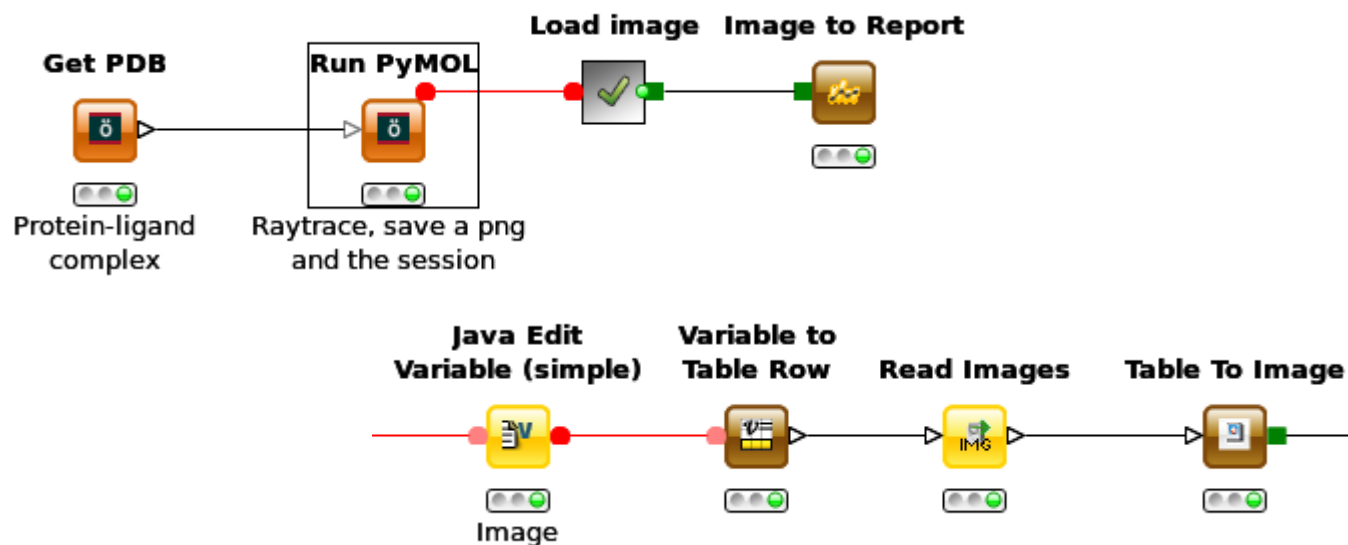
New Residue Scanning/Affinity maturation Node

- Node configuration with the same panel as in Maestro
 - Includes direct access to the online help
- Same look and feel as the other KNIME nodes
 - Cancel, Reset, Job control distribution ...
 - Batch execution



Reporting Nodes Improvements

- Pop-ups no longer block Run Maestro and Run Maestro command nodes and preference changes are now local
 - No change in these nodes will affect the other Maestro sessions
- Run PyMOL output files (log, structures, images...) can be used by downstream nodes and temporary files are cleaned up
 - Using %<flow_variable_name>% in the command script or %PyMOL_basename% added to the Variable Output

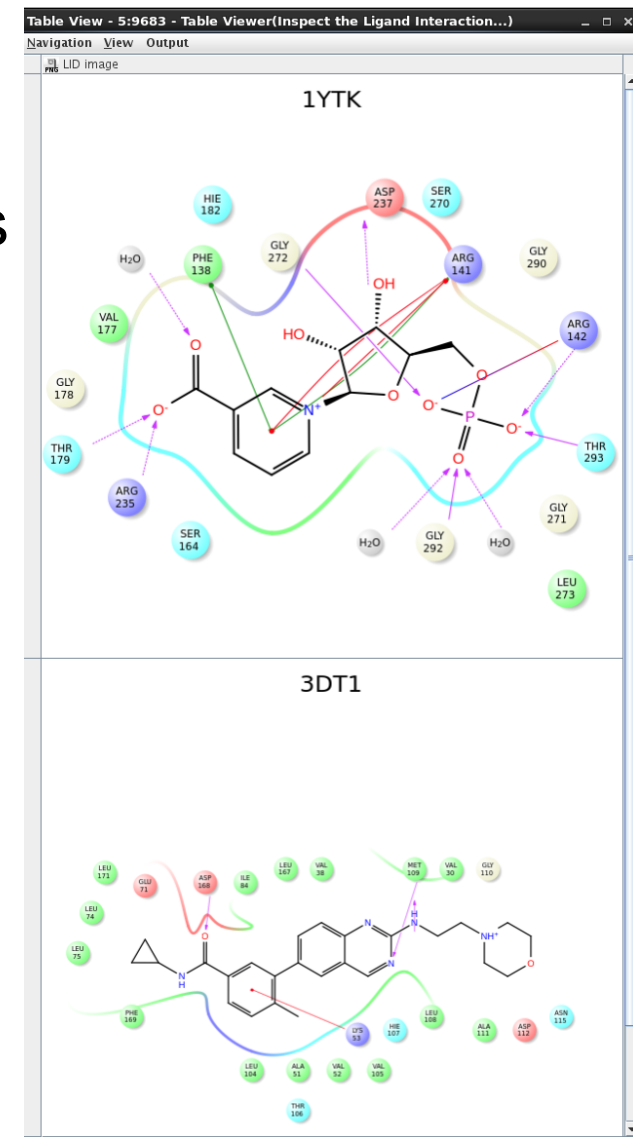
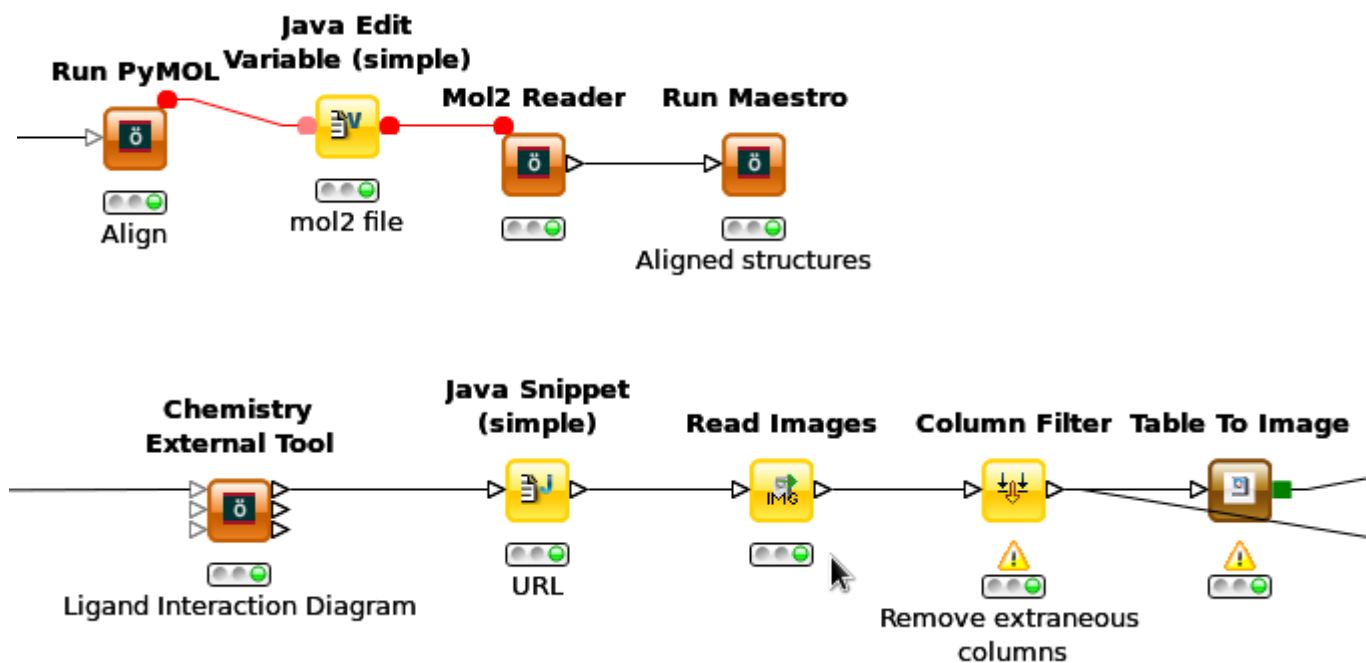


Main Fixes and Minor Improvements

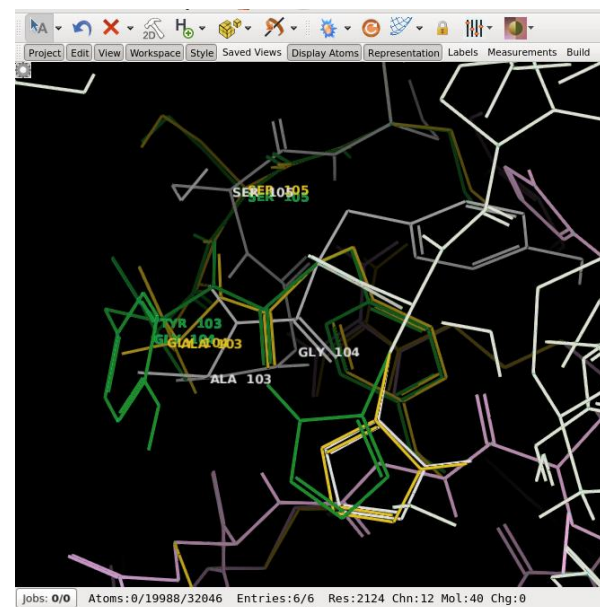
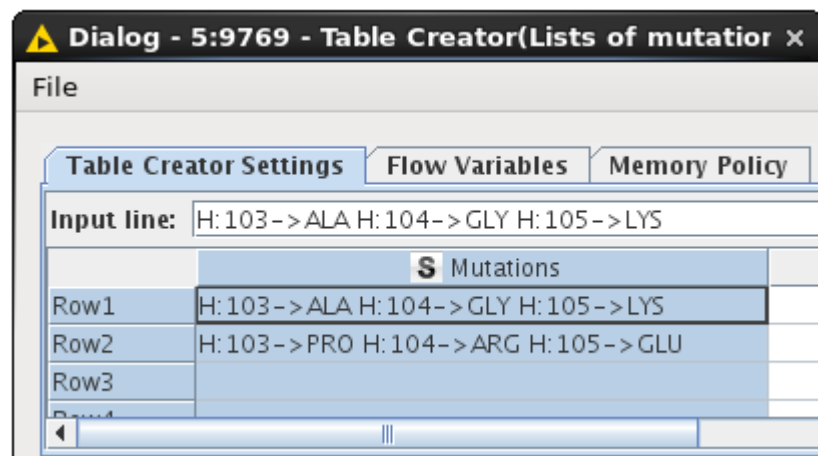
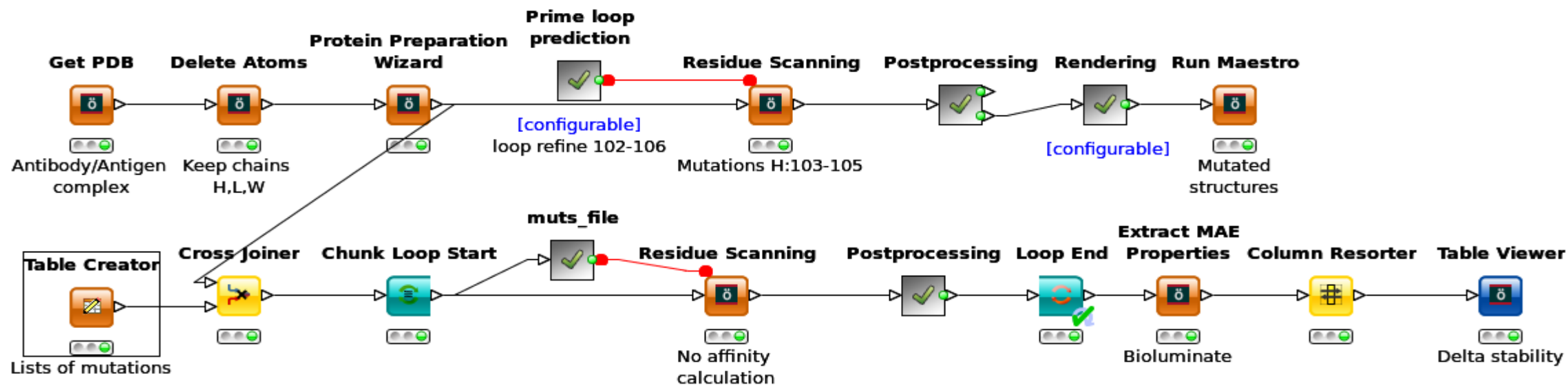
- Improved loading of the Schrödinger 's extensions during KNIME start-up
No more delay when the Licence server isn't responding
- Better control of Parameter flow variables in advanced scenarios
Use the “_rm_” keyword to remove an option with a value, while “_off_” can still be used if the argument doesn't have a value
- Most of the nodes use scripts from the distribution
 - eg RMSD, Desmond trajectory extract frames
 - No difference with the calculations run from Maestro
 - Take advantage of the latest improvements and fixes
- LigPrep no longer fails to write output in SDF
- Some nodes were fixed to run with UNC paths

New and Improved Workflow Examples

- Residue scanning – improvements and use the new node
- Run PyMOL – load rendered output image and structure files
- SiteMap binding site characterization – generate Ligand Interaction Diagrams



Residue Scanning/Affinity Maturation



Residue Scanning/Affinity Maturation

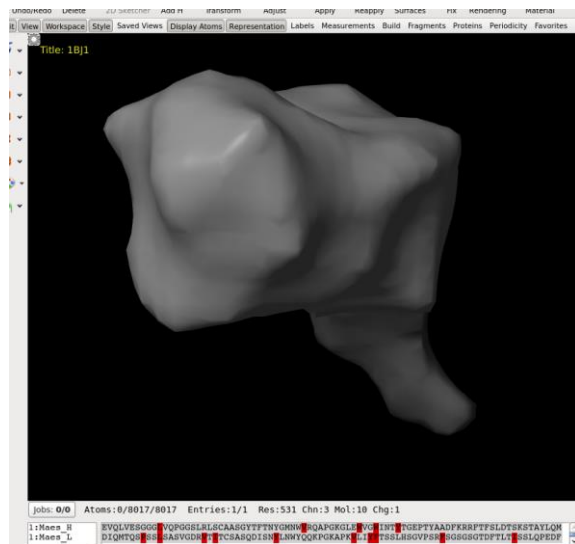
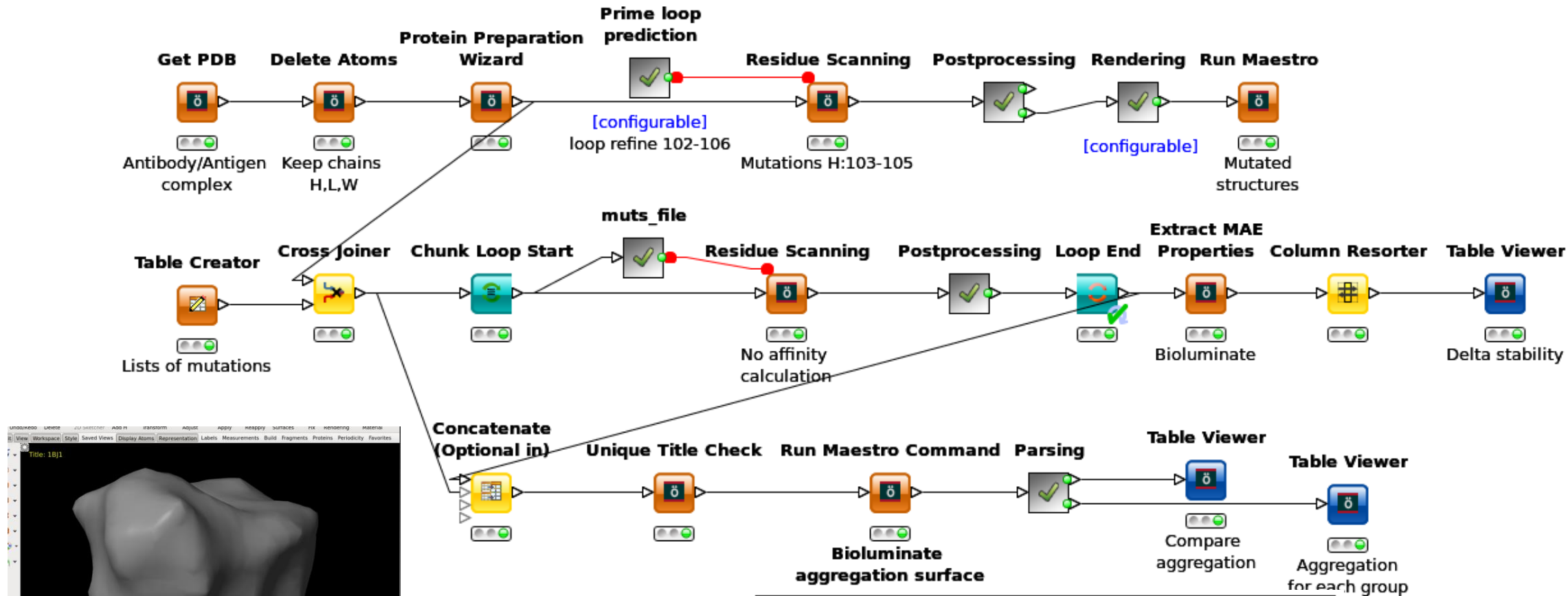


Table View - 6:9773 - Table Viewer(Compare)

| File | Hilite | Navigation | View | Output |
|--------|-----------|------------|-----------|-----------|
| Row ID | S Residue | D 0+Su... | D 1+Su... | D 2+Su... |
| Row12 | L:8 PRO | 10 | 10 | 10 |
| Row13 | W:46 ILE | 10 | 10 | 10 |
| Row11 | L:50 PHE | 9 | 8 | 11 |
| Row17 | W:85 PRO | 8 | 8 | 8 |
| Row9 | L:32 TYR | 7 | 7 | 7 |

2014-3 New Features

- Compatible with the latest version of KNIME (v2.10.0)
- A **configured Molecule reader** node is added **when dragging-and-dropping a Maestro file** into the workspace
- **Improved Simplified batch execution** and troubleshooting
- **Installation script improvements** to install Community Contributions and third-party extensions
- The 2D renderer is more stable on Linux
- Fixed a bug preventing several Glide grid generation nodes to be run in parallel
- Added an output port to the Setup Diagnosis node

[KNIME Schrödinger extensions 2.7]

KNIME 2.10 – some New Features

- The extensions are compatible with the latest version of KNIME (v2.10.0)
- It was released too late to be included in Schrodinger's installation (still KNIME 2.9.2)
- Find the full list on <http://tech.knime.org/whats-new-in-knime-210>
- New Nodes and New Features
 - GUI and Infrastructure
 - New Intro Page
 - **Auto Save**
 - Database
 - Database Connector Nodes
 - Database Table Selector
 - SQL Extract / Inject and Database SQL Executor
 - Database Sorter / GroupBy / Joiner
 - Social Media
 - Google and Twitter APIs
 - Data Manipulation
 - 7 new Distance Nodes
 - Moving Aggregation
 - Date/Time Shift, Time Series Missing Values

- Data Mining / Statistics
 - New View in Statistics Node
 - Time Series Analysis
- PMML
- Data Generation
- Textprocessing
- Image Import
 - Read Images, String to SVG

Improvements

- Data Manipulation
 - Column Rename
 - Normalizer , One2Many, and Many2One nodes
 - Cross Joiner
 - GroupBy, Pivoting, Rule Engine, and Column Aggregator
 - AutoBinner
- Data Mining
 - ROC Curve
- Open Street Maps Integration

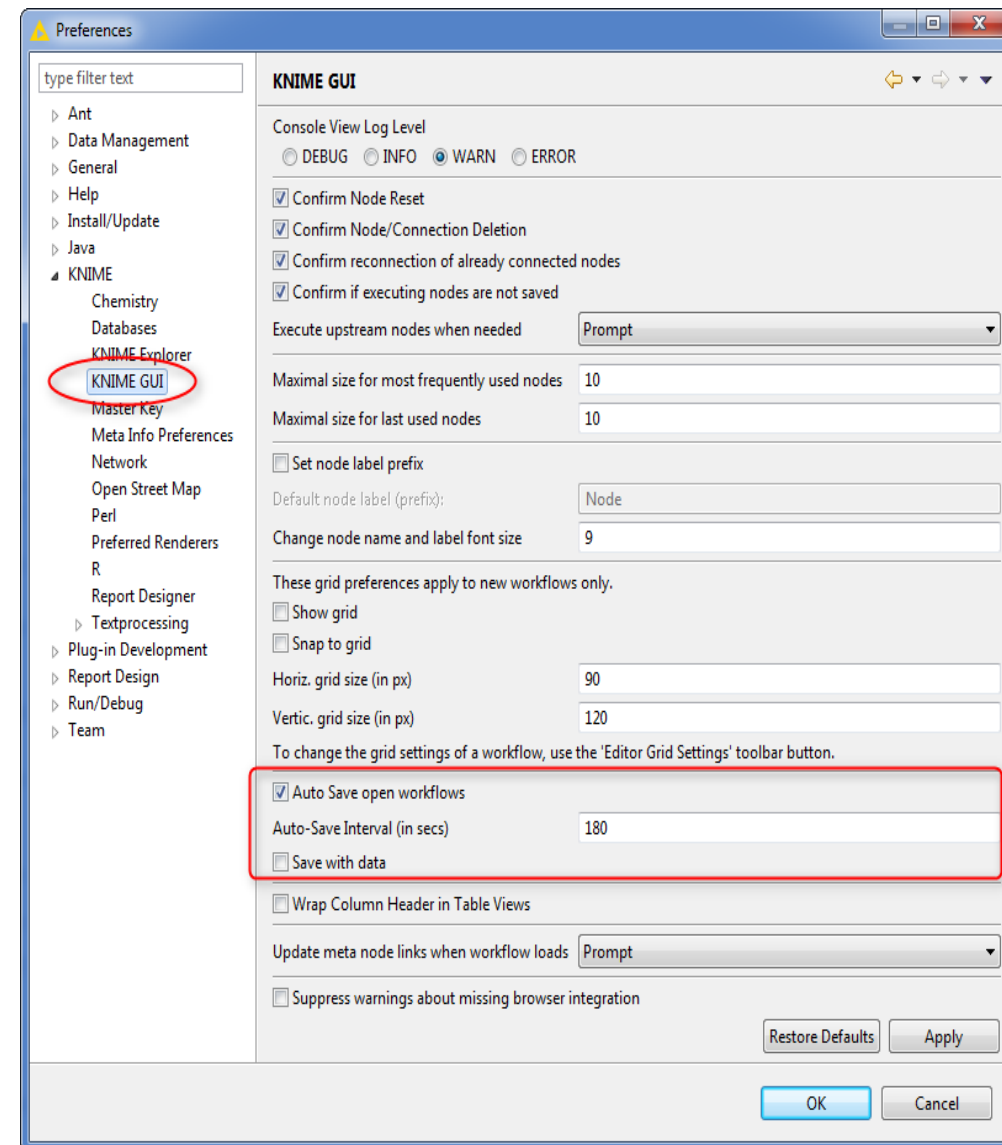
KNIME 2.10 – Auto-save

- **Auto-save**

If there is an unexpected break, your workflow will be recovered in the next KNIME session from the latest auto-save file. Disabled by default.

- **Java update consequence**

- On Windows, a re-installation of KNIME is required, due to the underlying Java update.
- On Mac or Linux, you can simply update your KNIME installation via the File menu.



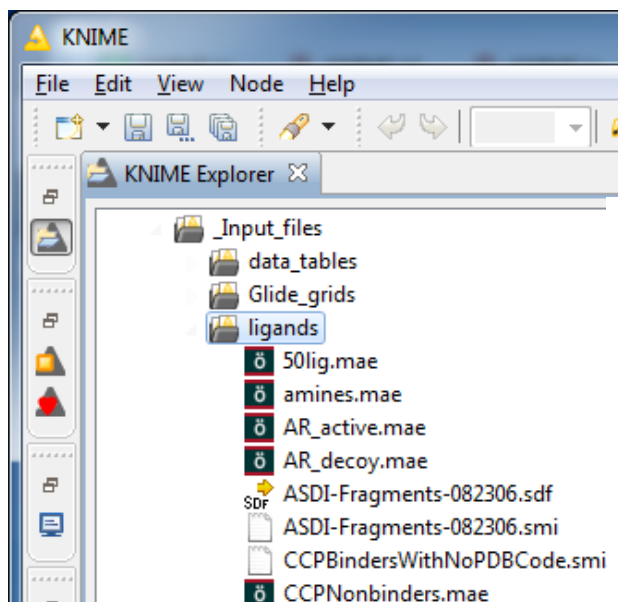
Molecule reader node from a dropped Maestro file

- A Molecule reader is added and automatically configured when dragging and dropping a Maestro file from a file explorer or the KNIME explorer view into the workspace.
- For the latter the files are stored in the workspace and the corresponding URL filename is eg:
knime://LOCAL/workflow_group/file.mae

These files are exported with the workflow or workflow group if they are located in the directory.

They can be organized and inspected directly from the KNIME explorer view.

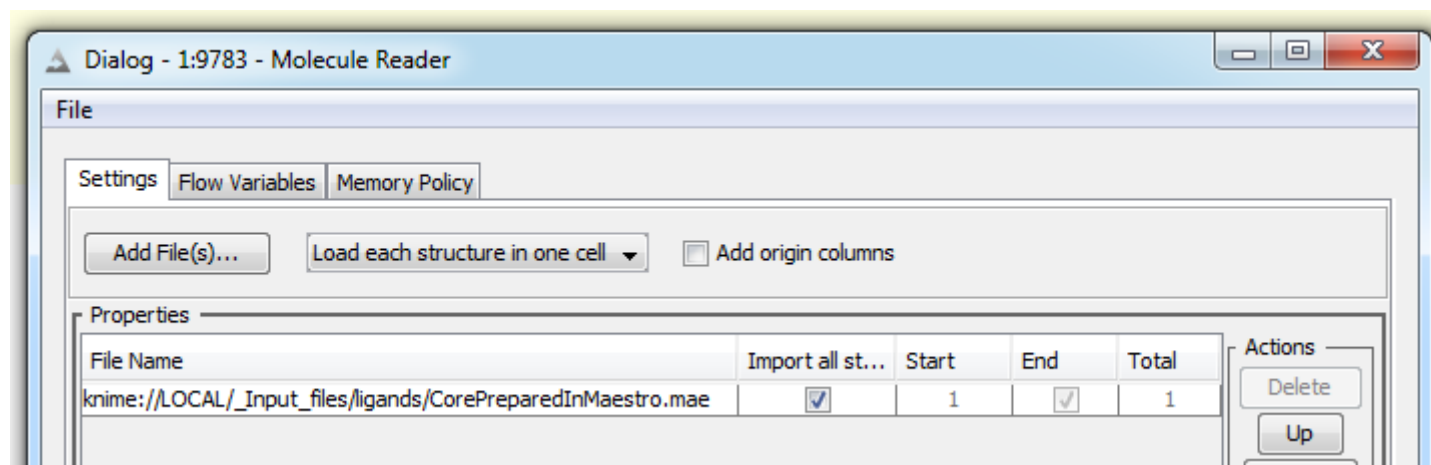
See the Pharmacophore > Shape screening first workflow example.



Molecule Reader



Node 1



Simplified Batch Execution Improvements

- Standardized the reader and writer node tag: %file%
The old tags are still supported
- Added support for several structure, Schrodinger types and Excel reader and writer nodes
- KNIME_batch.py -printcmd node list now includes:
 - the node annotation for Input and Output nodes
 - the node label for Quick Form nodes`-key <Name:$name, Label:$label> [Default:title]`

See the Pharmacophore > Shape screening and Docking > Virtual screening first workflow examples.

```
$SCHRODINGER/run -FROM maestro KNIME_batch.py -stdout INFO "D vs 1.zip" -run \  
-isdf /tmp/knime_workflow_example_data/ligands/fxa_ligands.sdf \  
-igrd /tmp/knime_workflow_example_data/Glide_grids/fxa_1f0r_AB_grids_recep \  
-osdf /tmp/DVS.sdf
```

Simplified Batch Execution – New Supported Nodes

- %file% Molecule Reader/Writer
Now the argument base name is -ostruct
- %file% SDF Reader/Writer
- %file% PDB, Mol2, Smiles Readers
- %file% Glide Grid Reader/Writer
- %file% Phase Hypothesis Reader/Writer
- %file% Sequence, Alignment Reader/Writer
- %file% Canvas Fingerprint Reader/Writer
- %file% CSV Reader/Writer
- %file% XLS Reader/Writer

See details with `–printallowed`

Keywords for workflows to be run in Maestro:

- %GUIsetting% Double, Integer, String Input QF
- %GUIsettingRADIO% String Radio Buttons QF
- %GUIsettingCOMBO% String Radio Buttons Quick form node
- %GUIsetting% File Upload Quick form node
- %selected entries% Molecule Reader
- %included entries% Molecule Reader
- %new group% Molecule Writer
- %maestro message% CSV Writer
- %maestro commands% CSV Writer

Start-up/batch Script Improvements

- Progress information in the terminal for easier debugging in batch:
 - **stdout** <min_log_level> Sets the minimum log level for the stdout ['DEBUG', 'INFO', 'WARN', 'ERROR', 'FATAL']
 - **stderr** <min_log_level> Sets the minimum log level for the stderr
 - **suppressErrors** Suppress the error window pop-up

On Windows it is in

C:\Users\...\AppData\Local\Schrodinger\appcrash\knime.log for now

- KNIME and Schrodinger options listed separately in the help message
Schrodinger options support relative path and KNIME's ones require absolute paths

See the Pharmacophore > Shape screening first workflow example:

```
$SCHRODINGER/run KNIME_batch.py "P Shape 1" -run -stdout INFO –  
suppressErrors...
```

Installation Script Improvements

- -features_list - any KNIME or third party features can now be installed in one go by specifying the complete list in the file
- -updatesites option - specifying a version number (like 2.9) will add both KNIME and Trusted Community Contributions web update sites
- -updatesites option supports comma separated list of update sites (can be both local zipped update site and web urls)

So -knime_updatesite was renamed into -updatesites and -knime_features_list into -features_list. The old option names are still supported.

- eg "\$SCHRODINGER/run" -FROM knime KNIME_install.py **-updatesite** 2.9,<http://tech.knime.org/update/community-contributions/2.7/> **-features_list** /path/to/feature.lst /path/to/myKNIMEinstallation/

With feature.lst file:

```
org.rdkit.knime.feature.feature.group
org.knime.features.quickform.feature.group
org.erlwood.knime.feature.feature.group (Lilly's nodes)
jp.co.infocom.cheminfo.marvin.feature.feature.group
com.vernalis.knime.feature.feature.group
```

See General > Installation workflow example and more details about the script in 2014-2 new feature slides.

Installation Script Improvements – use case

" \$SCHRODINGER/run" -FROM knime KNIME_install.py -verbose -updatesites 2.10,<http://tech.knime.org/update/community-contributions/2.7/> -features_list <see screenshot> -install_basechem 2.10 -schrod_updatesite /path/SchrodingerKNIMEUpdateSite_27006.zip <KNIME installation>

| | S Feature | S Version | S Feature name | S Excluded | S Update site | S Note |
|-------|---|----------------|--|------------------|---|--|
| Row0 | KNIME Nodes to create KNIME Quick Forms | 2.9.1.0041076 | org.knime.features.quickform.feature.group | | KNIME update site | |
| Row1 | KNIME Report Designer | 2.9.4.0042076 | com.knime.features.reporting.designer.feature.group | | KNIME update site | |
| Row2 | | | org.knime.features.ext.poi.feature.group | | KNIME update site | |
| Row3 | ChemAxon/Infocom Marvin Extensions Feature | 3.0135 | jp.co.infocom.cheminfo.marvin.feature.feature.group | | KNIME update site | |
| Row4 | KNIME Base Chemistry Types & Nodes | 2.10.0.0042428 | | org.knime.fea... | KNIME update site | Since there is already -install_basechem |
| Row5 | KNIME Chemistry Add-Ons | 2.10.0.0042428 | org.knime.features.ext.chem.tools.feature.group | | KNIME update site | |
| Row6 | KNIME Connectors for Common Databases | 2.10.0.0042821 | org.knime.features.dbdrivers.feature.group | | KNIME update site | |
| Row7 | KNIME Data Generation | 2.10.0.0042454 | org.knime.features.datageneration.feature.group | | KNIME update site | |
| Row8 | KNIME Decision Tree Ensembles | 2.10.0.0042428 | org.knime.features.base.treesensembles.feature.group | | KNIME update site | |
| Row9 | KNIME Distance Matrix | 2.10.0.0042807 | org.knime.features.distmatrix.feature.group | | KNIME update site | |
| Row10 | KNIME Ensemble Learning Methods | 2.10.0.0042872 | org.knime.features.ensembles.feature.group | | KNIME update site | |
| Row11 | KNIME External Tool Support | 2.10.0.0042738 | org.knime.features.ext.extool.feature.group | | KNIME update site | |
| Row12 | KNIME External Tool Support (Labs) | 2.10.0.0042428 | org.knime.features.exttool.feature.group | | KNIME update site | |
| Row13 | KNIME File Handling Nodes | 2.10.0.0042931 | org.knime.features.base.filehandling.feature.group | | KNIME update site | |
| Row14 | KNIME Google API Nodes | 2.10.0.0042599 | org.knime.features.google.api.feature.group | | KNIME update site | |
| Row15 | KNIME HTML/PDF Writer | 2.10.0.0042428 | org.knime.features.ext.birt.feature.group | | KNIME update site | |
| Row16 | KNIME Indexing and Searching | 2.10.0.0042431 | org.knime.features.ext.lucene.feature.group | | KNIME update site | |
| Row17 | KNIME Interactive R Statistics Integration | 2.10.0.0042974 | org.knime.features.r.feature.group | | KNIME update site | |
| Row18 | KNIME Itemset Mining | 2.10.0.0042428 | org.knime.features.ext.itemset.feature.group | | KNIME update site | |
| Row19 | KNIME JavaScript based nodes | 2.10.0.0043019 | org.knime.features.js.feature.group | | KNIME update site | |
| Row20 | KNIME JFreeChart | 2.10.0.0042428 | org.knime.features.ext.jfreechart.feature.group | | KNIME update site | |
| Row21 | KNIME JPMML Integration | 2.10.0.0042431 | org.knime.features.jpmmml.feature.group | | KNIME update site | |
| Row22 | KNIME LIBSVM Integration | 2.10.0.0042428 | org.knime.features.ext.libsvm.feature.group | | KNIME update site | |
| Row23 | KNIME Math Expression (JEP) | 2.10.0.0042428 | org.knime.features.ext.jep.feature.group | | KNIME update site | |
| Row24 | KNIME Neighborgram & ParUni | 2.10.0.0042428 | org.knime.features.neighborgram.feature.group | | KNIME update site | |
| Row25 | KNIME Network Mining | 2.10.0.0042983 | org.knime.features.network.feature.group | | KNIME update site | |
| Row26 | KNIME Network Mining distance matrix support | 2.10.0.0042428 | org.knime.features.network.distmatrix.feature.group | | KNIME update site | |
| Row27 | KNIME Open Street Map Integration | 2.10.0.0042433 | org.knime.features.ext.osm.feature.group | | KNIME update site | |
| Row28 | KNIME Optimization extension | 2.10.0.0042428 | org.knime.features.optimization.feature.group | | KNIME update site | |
| Row29 | KNIME Perl Integration | 2.10.0.0042428 | org.knime.features.ext.perl.feature.group | | KNIME update site | |
| Row30 | KNIME Pipeline Pilot Connector | 2.10.0.0042428 | org.knime.features.ext.webservice.client.pilot.feature.gr... | | KNIME update site | |
| Row31 | KNIME Python Scripting | 2.10.0.0042431 | org.knime.features.ext.jython.feature.group | | KNIME update site | |
| Row32 | KNIME R Statistics Integration (Windows Binaries) | 3.0.3.0042977 | org.knime.features.ext.r.bin.feature.group | | KNIME update site | |
| Row33 | KNIME Rule Viewer | 2.10.0.0042428 | org.knime.features.ext.md.feature.group | | KNIME update site | |
| Row34 | KNIME SAS7BDAT Reader (Windows only) | 2.10.0.0042428 | org.knime.features.ext.dsread.feature.group | | KNIME update site | |
| Row35 | KNIME Spotfire integration (Windows 32bit only) | 2.10.0.0042428 | org.knime.features.ext.spotfire.feature.group | | KNIME update site | |
| Row36 | KNIME SVG Support | 2.10.0.0042428 | org.knime.features.ext.svg.feature.group | | KNIME update site | |
| Row37 | KNIME Testing Framework | 2.10.0.0042871 | org.knime.features.testingapplication.feature.group | | KNIME update site | |
| Row38 | KNIME Twitter API Nodes | 2.10.0.0042599 | org.knime.features.twitter.api.feature.group | | KNIME update site | |
| Row39 | KNIME Virtual Nodes | 2.10.0.0042428 | org.knime.features.virtual.feature.group | | KNIME update site | |
| Row40 | KNIME Web Service Client | 2.10.0.0042428 | org.knime.features.ext.webservice.client.feature.group | | KNIME update site | |
| Row41 | KNIME Webanalytics | 2.10.0.0042730 | org.knime.features.webanalytics.feature.group | | KNIME update site | |
| Row42 | KNIME Weka Data Mining Integration (3.6) | 2.10.0.0042428 | org.knime.features.ext.weka.3.6.feature.group | | KNIME update site | |
| Row43 | KNIME Weka Data Mining Integration (3.7) | 2.10.0.0042428 | org.knime.features.ext.weka.3.7.feature.group | | KNIME update site | |
| Row44 | KNIME XML Processing | 2.10.0.0042428 | org.knime.features.xml.feature.group | | KNIME update site | |
| Row45 | RDKit | | org.rdkit.knime.feature.feature.group | | Trusted community nodes | |
| Row46 | RDKit | | org.rdkit.knime.wizards.feature.feature.group | | Trusted community nodes | |
| Row47 | Vernalis' nodes | | com.vernalis.knime.feature.feature.group | | Trusted community nodes | |
| Row48 | Lilly's nodes | | org.erlwood.knime.feature.feature.group | | http://tech.knime.org/update... | |

Setup Diagnosis Output

- Output port to report the results in an output table for post processing
- Output text file created (easily sent by email)
The file name and location is reported in the console and in the last column of the Output port.
- Reports whether KNIME is started through the startup script or as stand-alone

Setup Diagnosis Table Viewer



| Table View - 4:2 - Table Viewer(Diagnosis) | | |
|--|-------------------------------------|---|
| File | Hilite | Navigation View Output |
| Row ID | S Output | S Results File |
| Row0 | Schrodinger setup diagnosis results | /tmp/KNIME/SetupDiagnosis_9181507483831625025.txt |

Row: Row0 Column: Output Type: TextFileCell

File

Schrodinger setup diagnosis results

Checking required environments
SCHRODINGER = //home/data/schro-0B
LD_LIBRARY_PATH = //home/data/schro-0B/knime-v27010/lib/Linux-x86_64://home/data/schro-0B/mmshare-v27010/lib/Linux-x86_64:
ro-0B/mmshare-v27010/lib/Linux-x86_64:

Software versions
KNIME = 2.9.2
Schrodinger KNIME extensions = 2.9.2.v27010
mmshare = 27010

KNIME is started through startup script

Workflow runs in the Workbench

Checking knimeUtils library
The dynamic library knimeUtils is loaded successfully.

Checking KNIME_MAIN license
Schrodinger KNIME license has been checked out successfully.

Row: Row0
Column: Output
Type: TextFileCell

Close

Main Fixes

- Fixed a bug preventing several Glide grid generation nodes to be run in parallel
- The 2D renderer is more stable on Linux now it is run with a new mechanism
And it can be used in a stand-alone installation and no environment variable is required
- No more environment variable required to use the Chemistry external tool node in a stand-alone installation on Windows
- Zipped update site included in the Windows installers as well (as in Linux)

2014-2 New Features

- Includes the latest version of KNIME (v2.9.2)
- A **tool to automatically install** KNIME features and Schrodinger extensions in an existing installation
- The **Molecular Container Type** is supported in the Molecule to Mae node
- A **default renderer** can be selected for the Maestro columns in the Preferences
- New **Prime Energy** node
- Better calculation distribution in the **SiteMap** node
- A toggle button to operate on all the properties in the **Extract Mae properties** and **Set Maestro properties** nodes
- Additional formats that Maestro can import are supported in the **Molecule reader** node

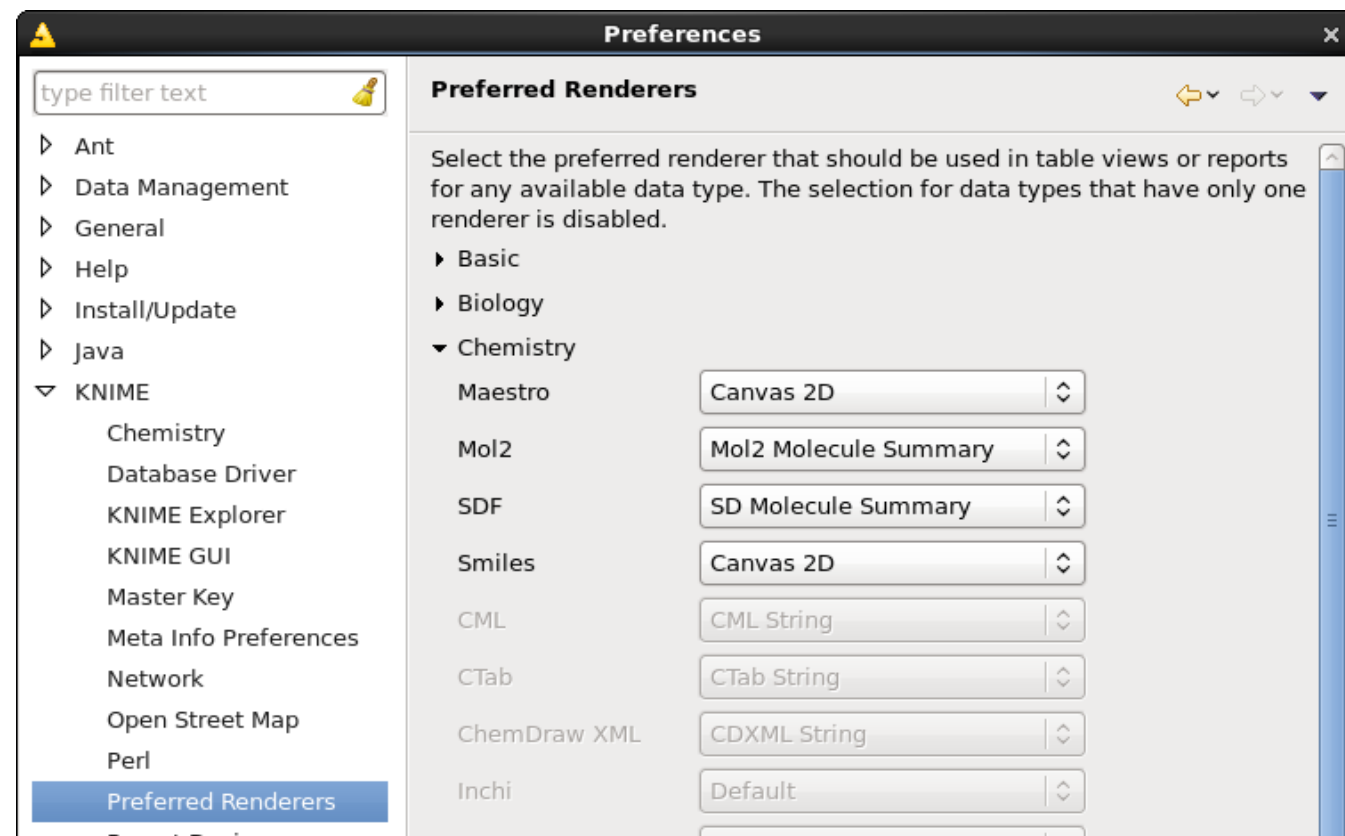
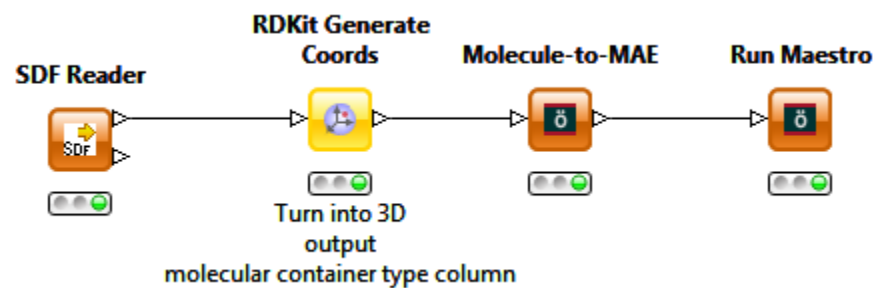
[KNIME Schrödinger extensions 2.6]

Installation Script

- A command line tool to automatically install KNIME features and Schrodinger extensions in an existing KNIME installation
- Available under https://www.schrodinger.com/KNIME_install/KNIME_install.zip and `$SCHRODINGER/knime-v*/python`
- `KNIME_install.py -schrod_updatesite (-install_basechem) -updatesites (-features_list)`
- eg to update the Schrodinger extensions in an existing Desktop KNIME installation:
`"$SCHRODINGER/run" -FROM knime KNIME_install.py -schrod_updatesite /path/to/SchrodingerKNIMEUpdateSite_26007.zip /path/to/myKNIMEinstallation/`
- eg to install the Schrodinger and a couple of other extensions in a fresh Desktop KNIME installation:
`"$SCHRODINGER/run" -FROM knime KNIME_install.py -install_basechem 2.9 -schrod_updatesite /path/to/SchrodingerKNIMEUpdateSite_26007.zip -updatesites 2.9 -features_list /path/to/feature.lst /path/to/myKNIMEinstallation/`
With feature.lst file containing for instance:
org.knime.features.quickform.feature.group
com.knime.features.reporting.designer.feature.group
org.knime.features.ext.poi.feature.group
(see the feature names in "Install New Software..." > "Install details")

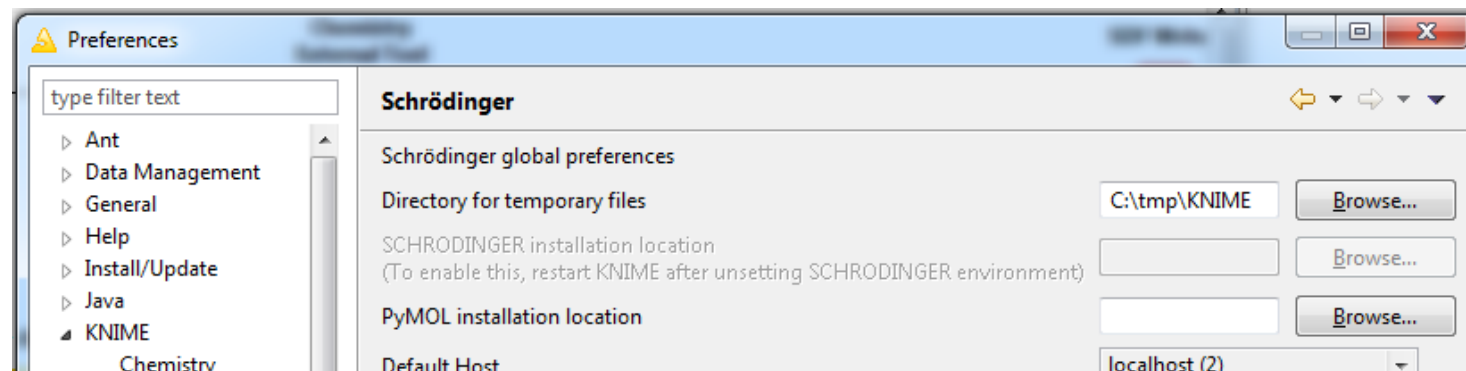
2D Renders and Molecular Container Type

- A default renderer can be selected for the Maestro column type in the Preferences
- The Molecule-to-MAE node supports the Molecular Container type
 - This is an Adapter cells that contains several representations of the same entity (eg SDF, CDK, RDKit...). So the conversion is performed only one time
 - It could be extended pretty easily to other nodes if needed



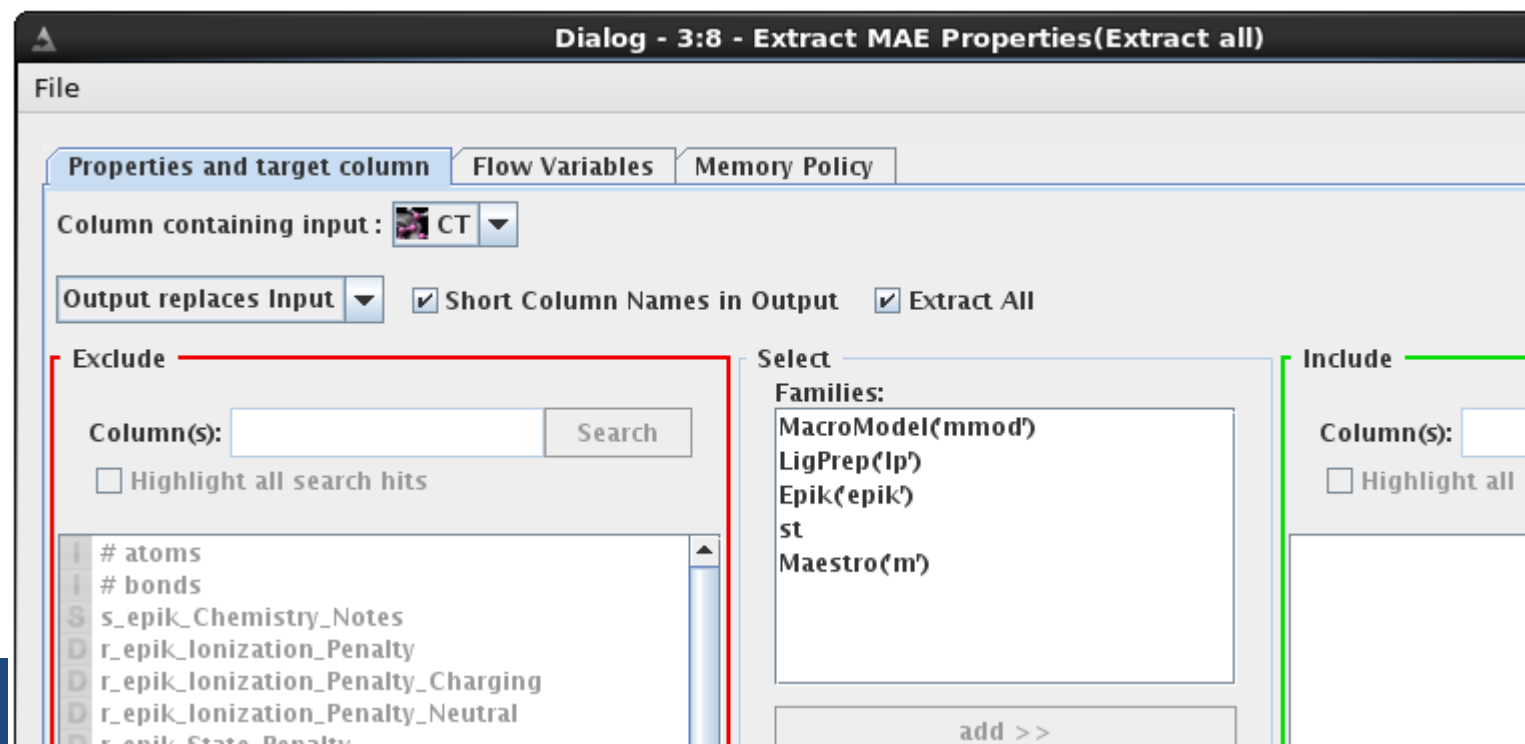
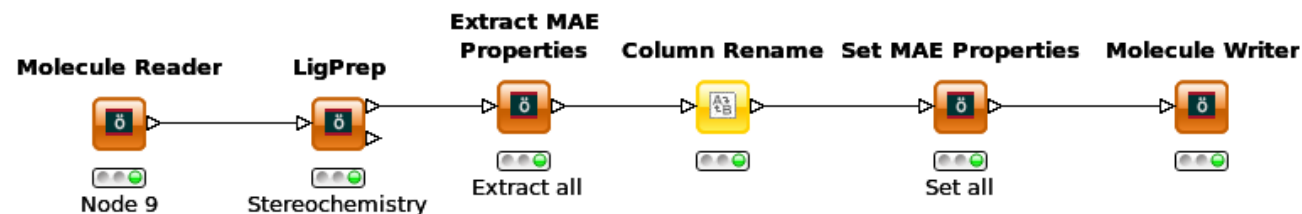
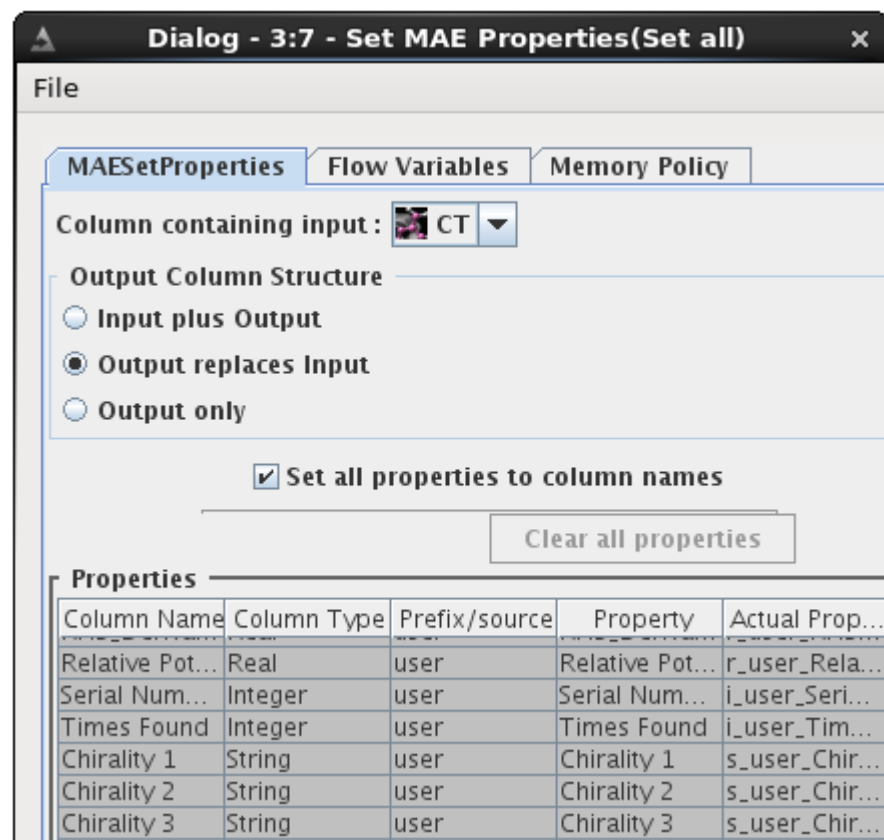
KNIME start-up script – accepts relative paths

- \$SCHRODINGER/knime : defines the required environment for the Schrodinger extensions in KNIME These can also be set in the Preferences
- Usual KNIME options are passed and some extra or simplified options; See the complete list using –help; They only affect the current session (eg computer specific settings)
- eg \$SCHRODINGER/knime -data Project/myWorkspace
 - maxHeap 1024m -maxThreads 3
 - schrodingerTempDir C:\tmp\KNIME -knimeTempDir C:\tmp
 - deleteTempFiles true
 - ooCmd Excel installation path/Open Office (oocalc)
 - (-batch)



Extract/Set MAE Properties – on all the properties

- Extract Mae properties – all of them
 - Useful when the generated properties can't be expected (eg LigPrep chirality information)
 - see also Extract properties: none, primary, all (eg in Glide ligand docking node)
- Set Mae properties – all

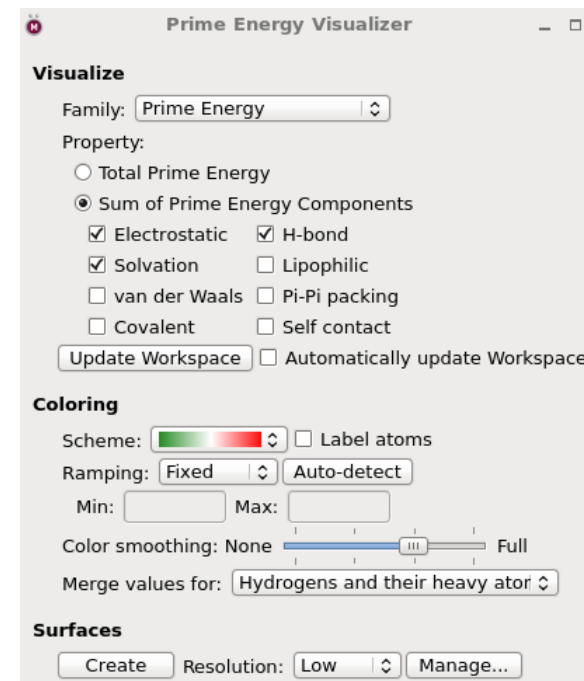
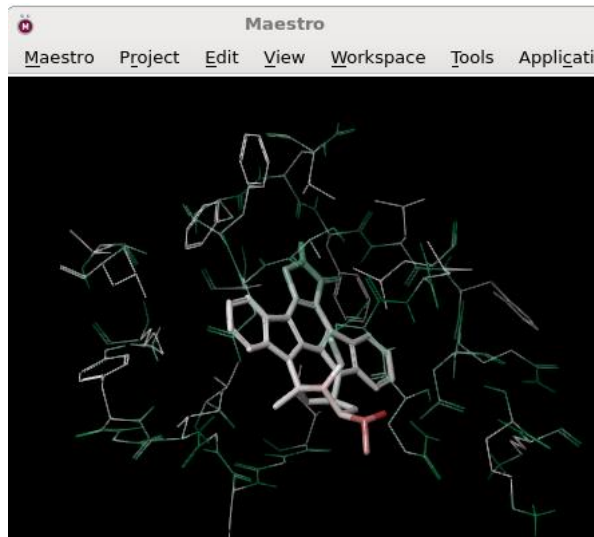
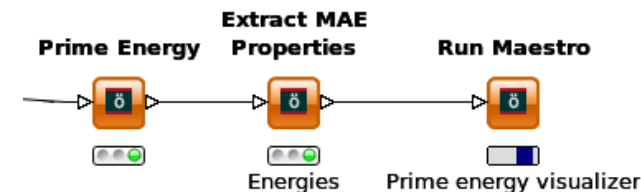


Other Nodes

- SiteMap – better calculation distribution
See in the SiteMap.in : PROT sitemap_<>_in_1.mae,sitemap_<>_in_2.mae
- Prime energy – new node
- Split by structure – support the parameter flow variables
eg SplitStruct-merge_ligands_with_chain = “_on_”

Robustness

- Setup Diagnosis – ensure scratch directories are writable,
no schrodinger.host file interference



Main Fixes

- MacroModel nodes etc – expose the force field selector again
 - OPLS 2.1 isn't exposed though and only accessible using the parameter flow variable.
- Chemistry external tool- Add support to mol type
- Molecule writer- column containing output file name- add .mae if missing
- ConfGen- generated only one conformation per structure

2014-1 New Features

- Includes the latest version of KNIME (v2.9)
- Can use any command line option not exposed in the **Glide ligand docking** node configuration panel
- Can use a specific template in the **Prime Build Homology Modeling** node
- Can operate more easily on the structures passed to the **Run PyMOL** node

KNIME 2.9 – Some New Features

<http://tech.knime.org/whats-new-in-knime-29>

- **Column Selection Framework Extended and Improve**

New Selection Criteria in **Column Filter** Node and similar nodes

The Column Filter configuration window now allows to select the input data columns: manually, by type, by name based on a RegEx / Wildcard expression

- **Rule Based Framework Extended and Improved**

New Rule Engine Node, Rule Engine Variable, Rule Based Row Filter/Splitter

- **Workflow Monitoring,, and Administration**

- **Send Email** (new node)

The Send Email node sends an email to a given email address. It can be used to send updates about the workflow execution status.

- **Save Workflow** (new node) Performance

- **Save As ...** <under a different name> (New File Menu Option)

- **Easier Extension Installation**

All existing KNIME update sites are now available in the Preferences menu item (File -> Preferences -> Install/Update -> Available Software Sites).

- **Context Extractor Node** (new node)

The node Extract Context Properties makes some workflow context related properties available at the variable output port, including current user name, workflow name, and working directory.

KNIME 2.9 – Some New Features

- Data Generation

- Counter Generation (new node)

The Counter Generation node adds a counter column to the input data table. The counter starting point (Min. Value) and the step size (Scale Unit) can be defined in the configuration window.

- Better Model Training and Evaluation

- Unified Format for Predictor Nodes, Extended Linear Regression Output, Numeric Scorer

- Other New Features and Nodes

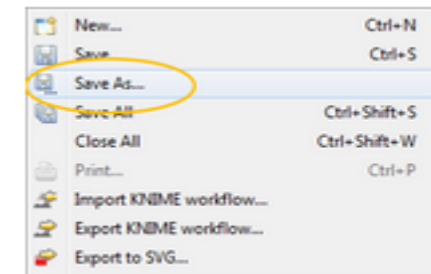
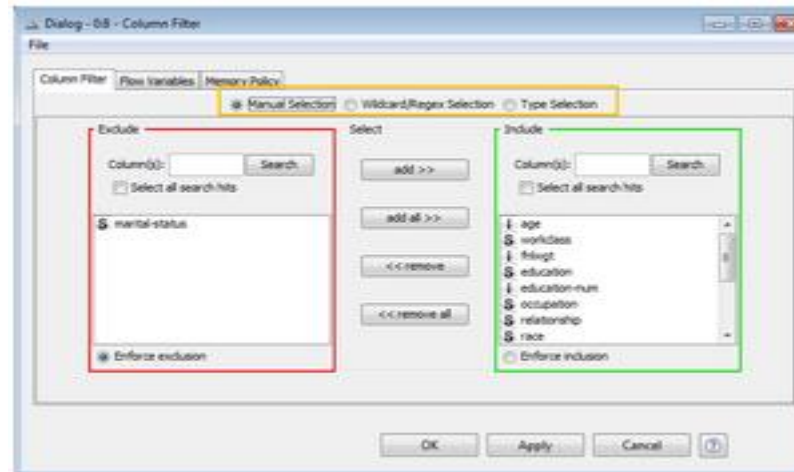
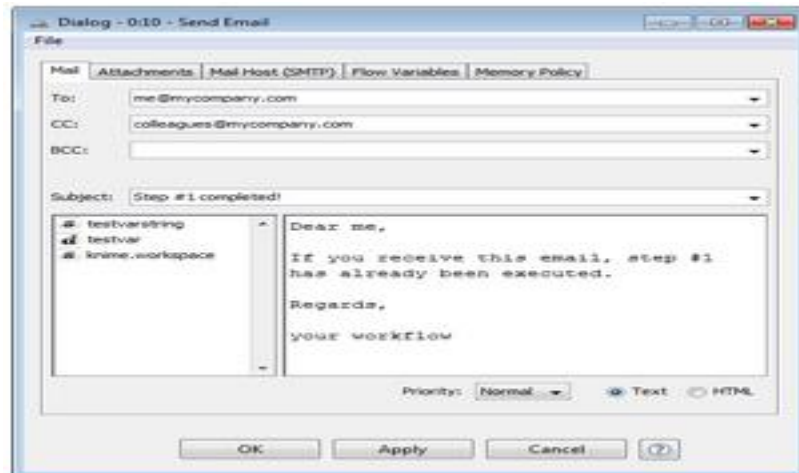
- Cross Joiner (new node)

Performs a cross join of two tables. Each row of the first table is joined with each row of the second table.

- Pair Extractor (new node)

"Unpivot" a distance matrix by extracting all pairwise distances from a distance matrix column.

- Flow Variables and Missing Values



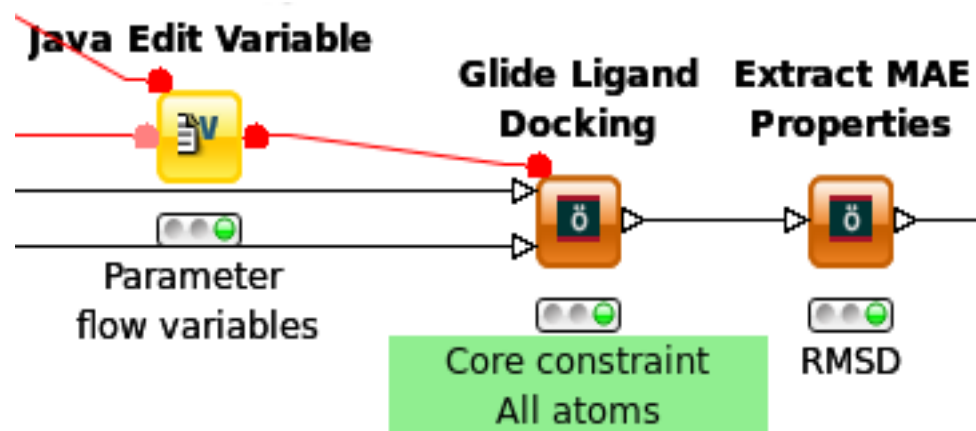
Glide Ligand Docking

- Can use any Glide Simple Input file option not exposed in the configuration panels
- Through Parameter flow variables
- Options list: glide_sif.py -help
- eg Core constraints:

GlideLigandDocking-ref_ligand_file = <path/file.mae>

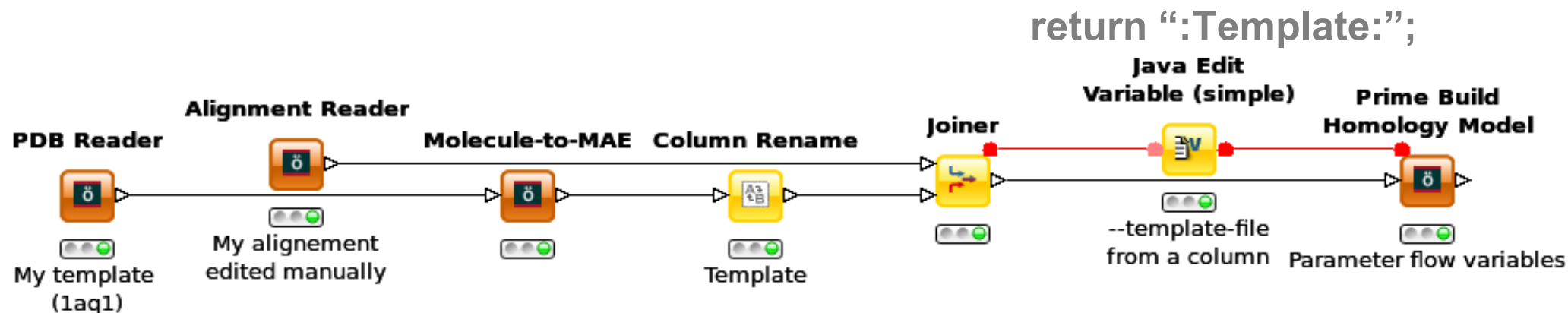
GlideLigandDocking-use_ref_ligand = yes

```
.../tmp/KNIME/knime_scripts_..._19009/glide_sif.py -forceplanar false -gridfile /tmp/recep.zip ... -poses_per_lig 1 ... -ref_ligand_file /tmp/ref.mae -  
use_ref_ligand yes
```



Prime Build Homology Modelling

- Can use a specific template
- Via a parameter flow variable:
PrimeBuild--template-file pointing to the file or the column containing the template.



Joined table - 2:9643 - Joiner

| Table "default" - Rows: 1 | | | Spec - Columns: 2 | |
|---------------------------|--------------------------|-------------------------------|-------------------|--|
| Row ID | Alignment | Template | | |
| Row0 | Alignment: #sequences... | Molecule: myTem #atoms: 23... | | |

KNIME in Batch Wrapper

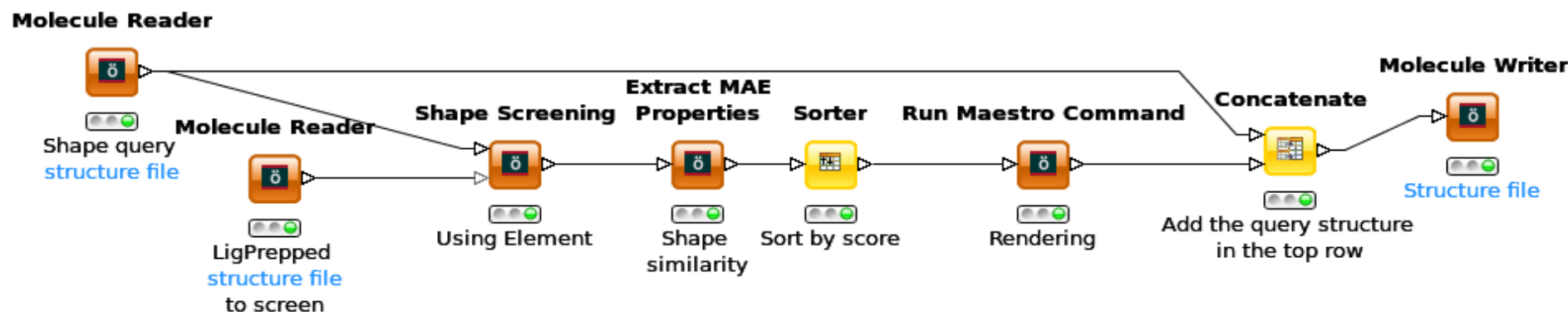
- KNIME in batch wrapper – list the allowed nodes and corresponding tags `$SCHRODINGER/run KNIME_batch.py <workflow.zip|workspace/workflow> -printallowed`

| Text | Node | Action |
|------------------------------------|---|---|
| Structure file | Molecule Reader | Read the first file specified in the node. |
| Selected entries (Maestro only) | Molecule Reader | Read the entries that are selected in the Project Table. |
| ... | | |
| Text file | CSV Writer | Write the output to specified file. |
| GUIsetting | Double Input, Integer Input, String Input | Add a text box control to the panel and assign the value that is set in the text box. |

- printusage, -printcmd, -run, -GUI options (already in 2013-1)

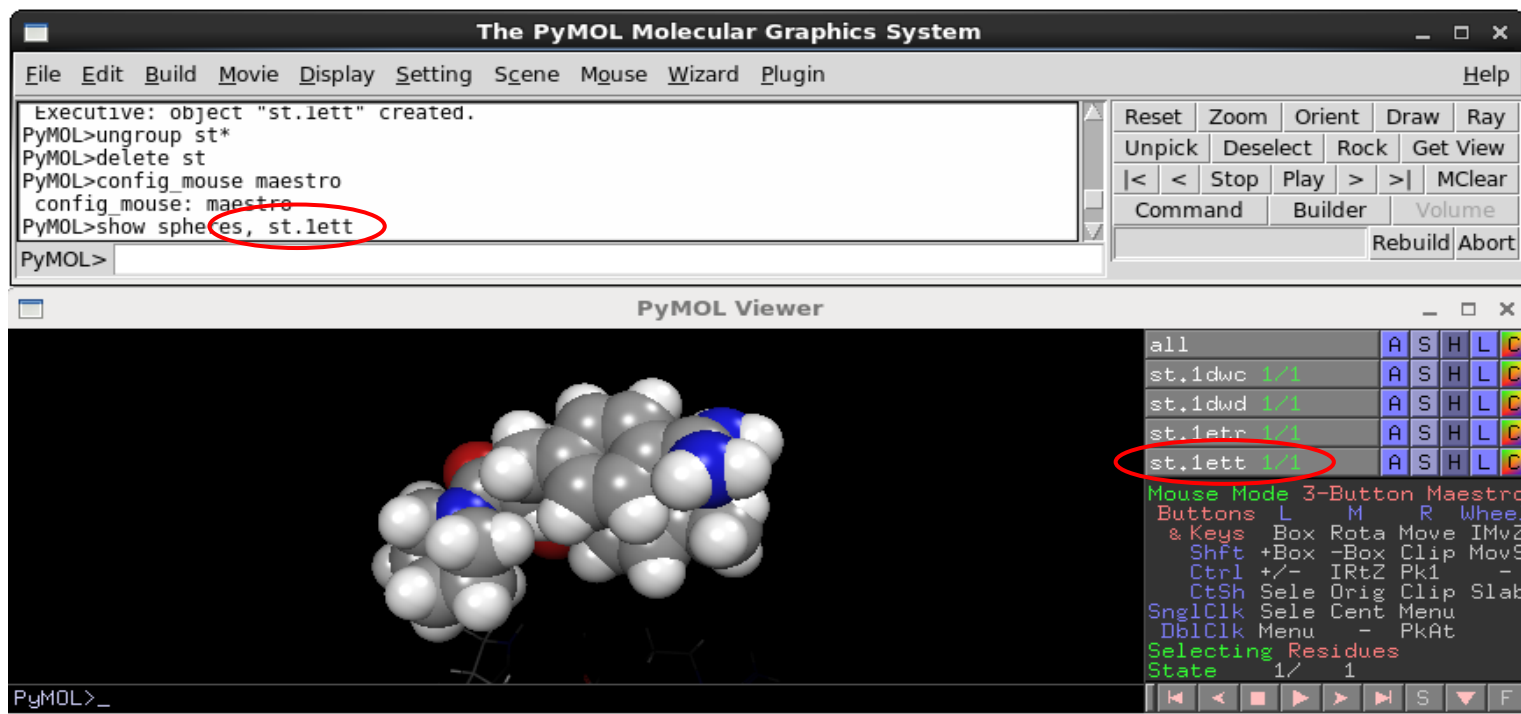
See Shape screening workflow example:

```
$SCHRODINGER/run KNIME_batch.py P\ Shape\ 1.zip -run -imae /tmp/fragments.mae -imae1 /tmp/Query.mae -omae /tmp/PhaseShape.mae
```



Run PyMOL, Run Canvas

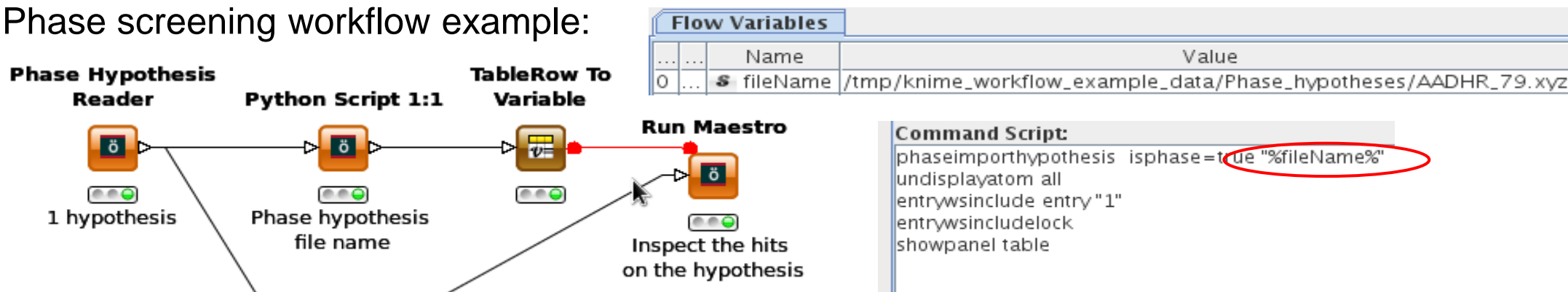
- Run PyMOL
 - Structures ungrouped to operate more easily on the structures
 - Disabled when the workflow is executed in batch mode
- Run Canvas
 - Disabled when the workflow is executed in batch mode



Miscellaneous

- Flow variables can be used in the Run Maestro node script (and already in Run Maestro command)

See the Phase screening workflow example:



- Parameter flow variables can be used for ConfGen
- Chemistry External Tool- cms as allowed input and output types

Important bug fixes:

- Glide ligand docking – when multiple poses saved
- Extract mae properties – blank lists

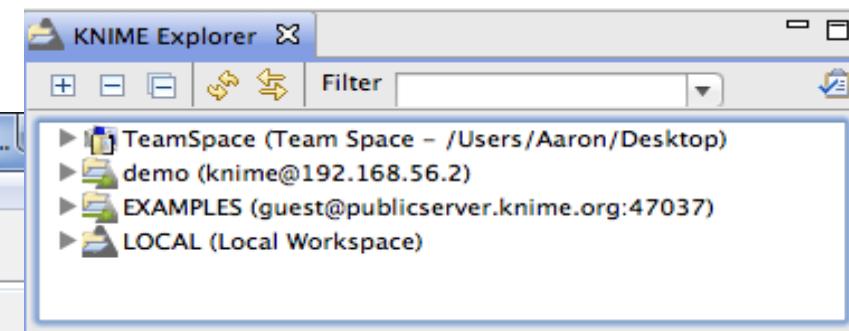
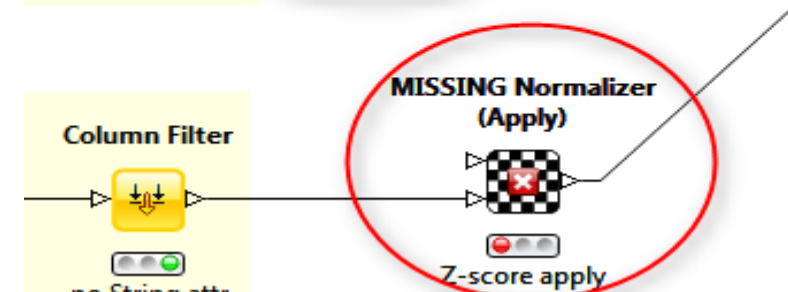
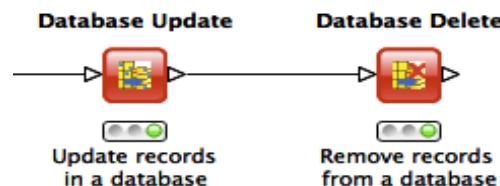
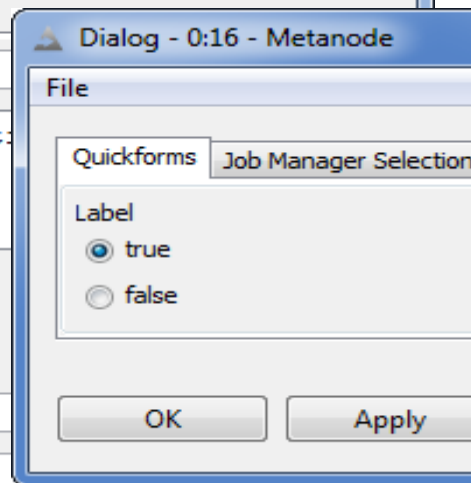
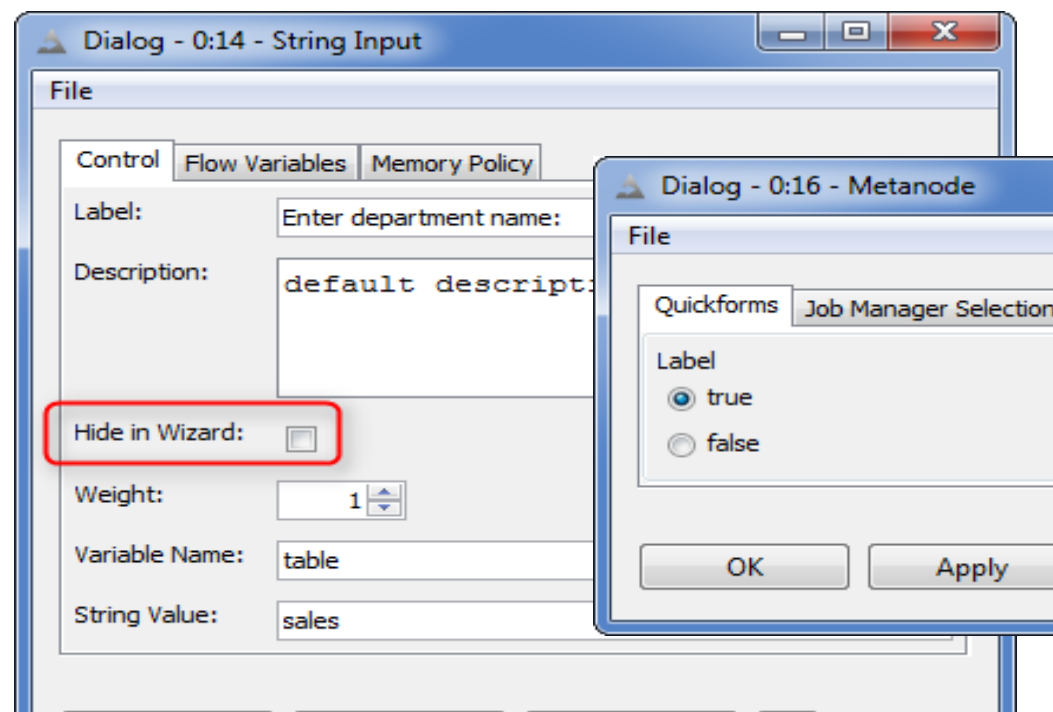
2013 new features

- Ease of use
 - Stand-alone **installation configuration** in the Preferences
 - Improve the **compatibility** with other provider nodes (less conversions)
 - Mine the **list of the workflows and nodes** in a workspace
 - **Batch command generation** – based on workflow annotations
- Functionalities:
 - Use backend **option not exposed in the configuration panels**
 - **SiteMap, PyMOL, Glide grid writer** new nodes
 - **Easier prototyping** with the new Chemistry External Tool node
- Integration:
 - Run KNIME workflows **from Seurat**
 - Can invoke **web service** to execute LigPrep node. Execute some Schrödinger backends through the Generic Web Service Client node

Some KNIME 2.6 and 2.7 new features

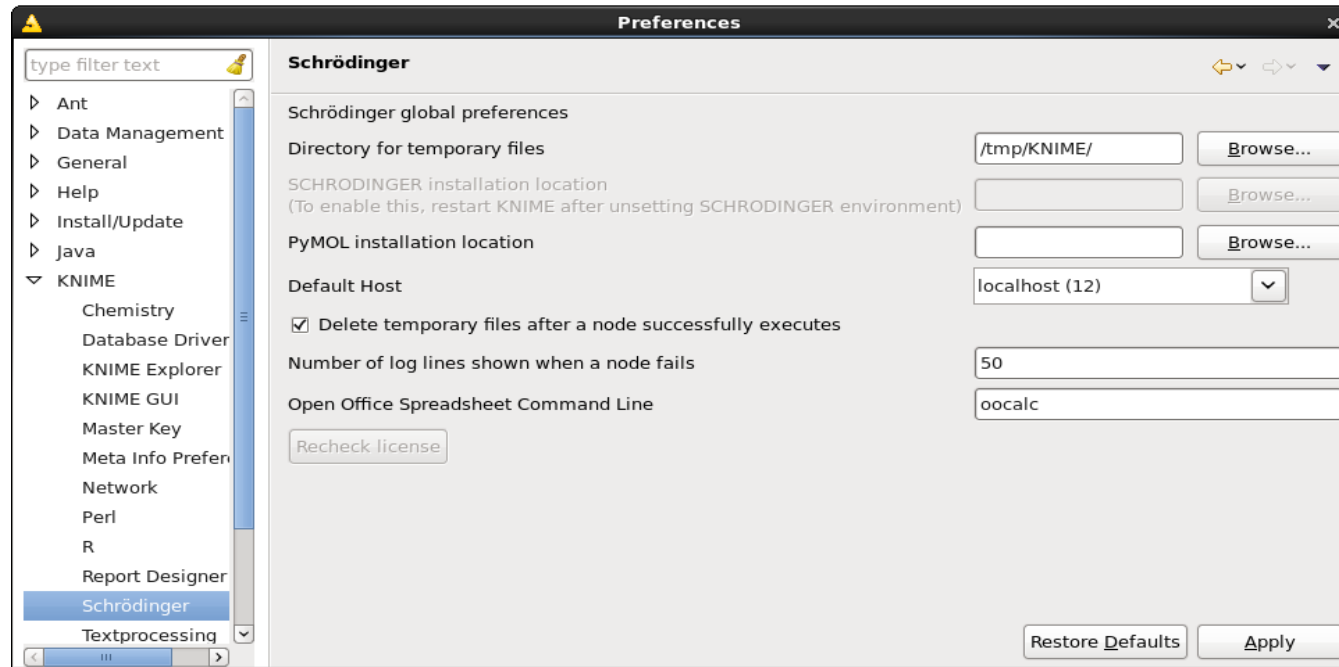
<http://tech.knime.org/whats-new-in-knime-27>

- Random forest node
- Metanode – add/remove/reorder ports
- Grid layout and snapping
- Improved String Manipulation and Java Snippet nodes
- New database nodes:
- New quick form nodes:

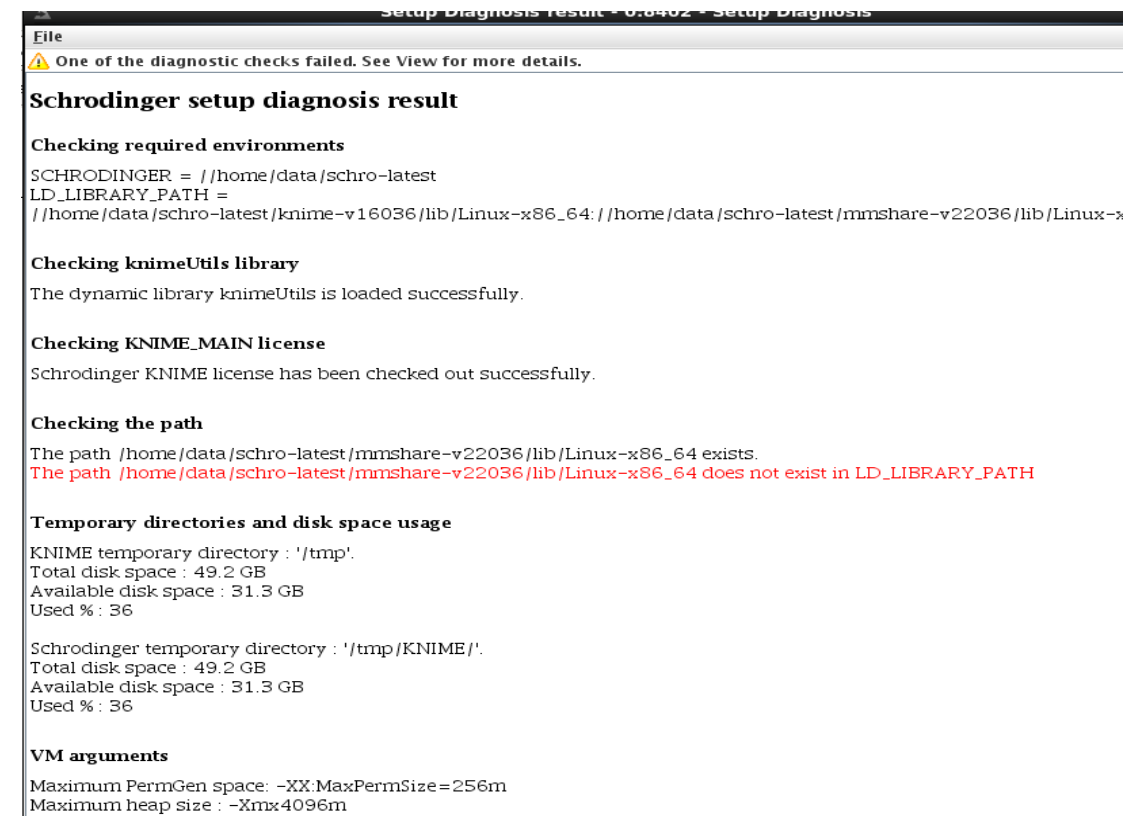


Environment configurable in the preferences

- For a stand-alone installation
- Other ways (\$SCHRODINGER/run, start-up script, hunt based)



- **Set-up diagnosis** node for the KNIME Server
 - Environment, scratch directories
 - License, Backend installed



Batch command generation

- Command line to be run in batch generated **based on node annotations**

Similar to the KNIME in Maestro ones eg “**Structure file**” for Molecule reader and writer nodes

eg \$SCHRODINGER/run KNIME_batch.py QM.zip **-printcmd**

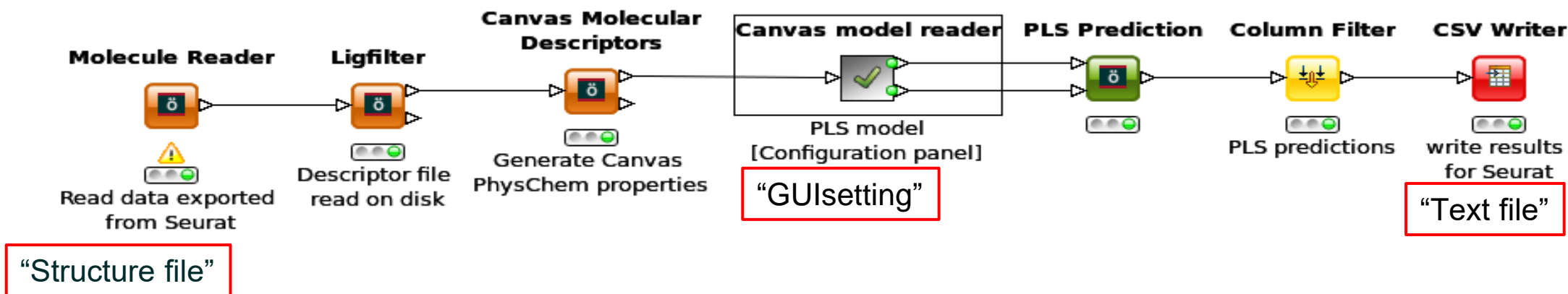
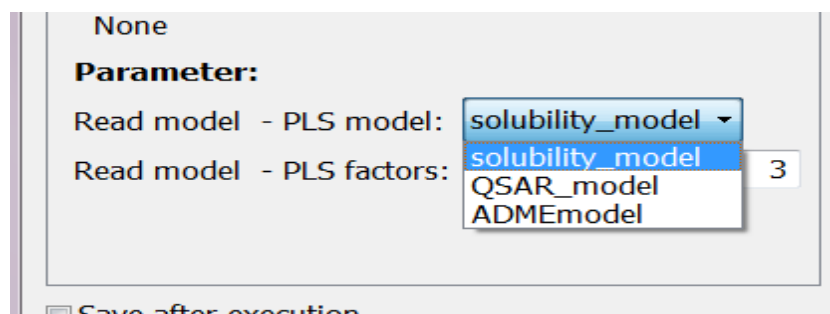
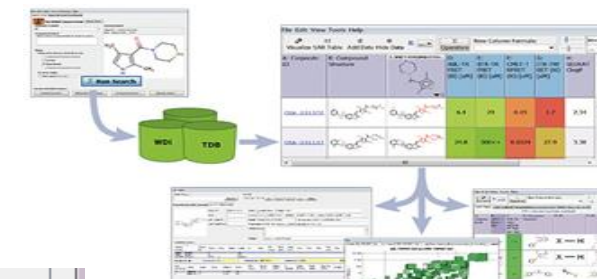
```
$SCHRODINGER/knime -batch -nosave -maxThreads 1 -nosplash -workflowFile=QM.zip
```

```
-option=8380,DataURL/0,/tmp/Aniline.smi,String
```

```
-option=8386,output_file_name,/tmp/QMprotocolOutput.mae,String
```

```
-option=8399,value/value,localhost:2,String
```

- Workflows easily run in **Seurat**

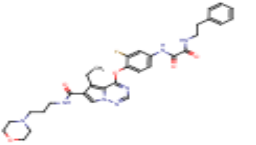
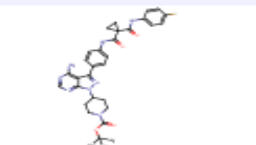
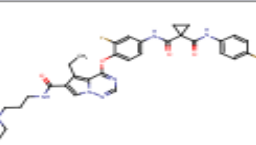
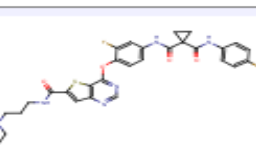


KNIME in Seurat

Assay Display (cmetMain)

File Edit View Tools Help

Visualize Trellis Pie Chart SAR Table Add Data Hide Data Σ 11 Operators New Column Formula:

| A: Corporate ID | B: Compound Structure | C: BTK-TRFRET (Ki) [uM] | D: CMET-TRFRET (Ki) [uM] | E: ITK-TRFRET (Ki) [uM] | F: H-Bond Acceptors | G: H-Bond Donors | H: Select Chemist (Pic List) |
|----------------------------|---|-------------------------|--------------------------|-------------------------|---------------------|------------------|------------------------------|
| CRA-033905 |  | 5,0 | 70 | 0,76 | 11 | 3,0 | |
| CRA-033223 |  | 5,7 | 0,072 | 140 | 11 | 3,0 | |
| CRA-033660 |  | 25,3+ | 0,0143 | 26,6 | 11 | 3,0 | |
| CRA-034275 |  | 58 | 0,061 | 60 | 11 | 3,0 | |

Suchen: Nächste suchen Vorherige suchen Groß-/Kleinschreibung

R0/C4 285 rows 7 cols / filtered: 0 rows / hidden: 0 rows 0 cols

Add Data

Databases to Search

pri

Properties

- Seurat-Built-In
- ChemAxon libMCS
- JChem
- Schrodinger
- KNIME
- KNIME2
 - Knime Example 3
 - Knime Example 4
 - Knime Docking 3c
- New Prop
 - hERG Binder
 - ACDLabs logS (mol/l)
 - ACDLabs logS (uM)
 - Lipinski Filter
 - Lipinski Score
 - Veber Filter
 - QSAR - CaCO-2 Cell Permeability
 - QSAR - Human effective permeability

Search: Type here to filter names

Add Close

Parameter flow variables

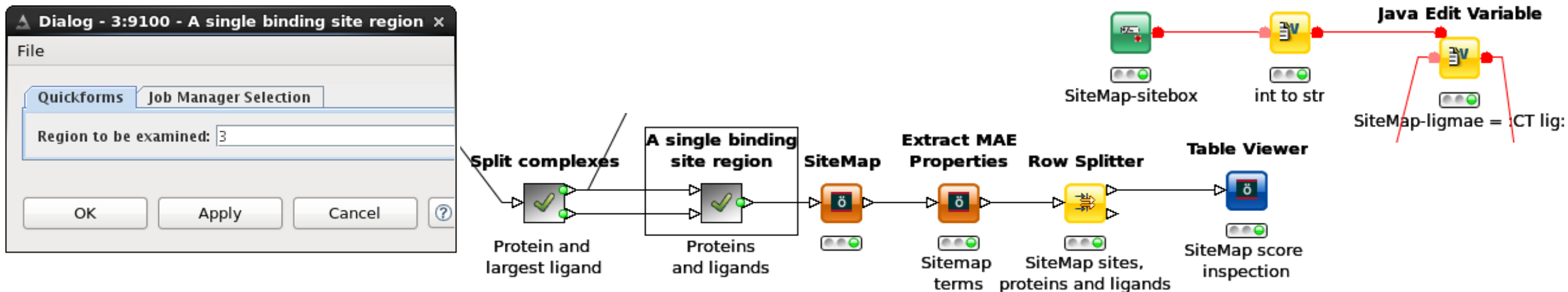
- **Any backend command line option** not exposed in the node configuration panel
- Value, activate, value/structure from an input column, extra output column
- Metanode GUI with the Quick form nodes

eg SiteMap-sitebox = 3 SiteMap-ligmae = :CT lig:

Sitemap -HOST localhost:4 -j sitemap_-732349751_1 -maxsites 5 -modphobic 3 -keeplogs no

-sitebox 3 -ligmae sitemap_-732349751_in_1_CT_lig.mae -prot sitemap_-732349751_in_1.mae

- The console reads: Detected a SiteMap flow variable: SiteMap-sitebox=3 ...



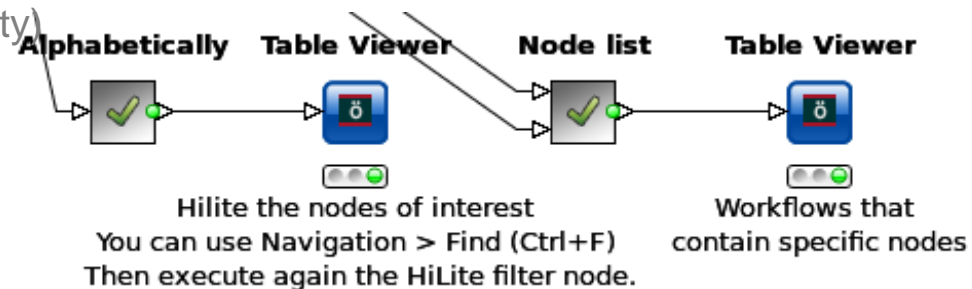
- Glide ligand docking, Prime nodes, Protein preparation wizard, SiteMap, some Jaguar, MacroModel and Canvas nodes. **Simple to activate** for other nodes when needed.

Workflow examples and Workflow list node

- Workflow examples available as a workspace under \$SCHRODINGER/knime-v.../tutorial/
- Workflow list node** (free, in a separate plugin feature)

Lists the nodes and workflows in the workspace

- Latest modified workflows
- workflows containing specific nodes (eg example to create a new one)
- Compare several versions of a workflow (date, complexity)
- Find a workflow buried in groups
- Workspace clean up (size on disk)



View - 5:195 - Table Viewer(Hilite) - □ x

Navigation View Output

| S Name | I Coun... |
|-----------------------------|-----------|
| Cell Replacer | 5 |
| Cell Splitter | 326 |
| Cell Splitter By Position | 13 |
| Cell To PMML | 2 |
| Chemistry External Tool | 57 |
| Chemistry External Tool 0:1 | 114 |
| Chemistry External Tool 1:1 | 668 |
| Chemistry External Tool 1:2 | 91 |
| Chemistry External Tool 2:1 | 61 |
| Chemistry External Tool 2:2 | 110 |
| Chunk Loop Start | 49 |
| Cluster Assigner | 1 |
| Color Appender | 4 |

Output data - 5:299:298 - Column Resorter

4

Spec - Columns: 6

Properties

Flow Variables

| | S Workflow group | S Workflow name | S Last modification ... | D Size (i |
|--------------------|----------------------------------|----------------------------------|--------------------------------|------------------|
| ternal Tool 0:1(1) | \$\$ | Schodinger license diagnostics X | 2012-10-05 08:37:... | 0.012 |
| ternal Tool 0:1(1) | Customer / Molecular mechanics | MMod scan [Antonio, 101280] X | 2012-10-05 08:29:... | 1.649 |
| ternal Tool 0:1(1) | Examples / Molecular dynami... | MD simul 1 [5.0] | 2012-12-27 10:08:... | 1.964 |
| ternal Tool 0:1(1) | Examples / Molecular dynami... | MD simul 1-2 [5.0] | 2012-12-27 10:08:... | 21.745 |
| ternal Tool 0:1(1) | Examples / Molecular dynami... | MD simul 1-3 [5.0] | 2012-12-27 10:08:... | 26.568 |
| ternal Tool 0:1(1) | Examples / Quantum mechani... | QM pKa (5.0) | 2012-11-15 09:09:... | 0.426 |
| ternal Tool 0:1(1) | Examples- new / Cheminform... | 12 | 2012-10-05 08:25:... | 4.037 |
| ternal Tool 0:1(1) | Internal / Tools / Check KNIM... | KNIME_WinInstCheck_OLD1 | 2012-10-05 08:38:... | 0.517 |
| ternal Tool 0:1(1) | Internal / Tools / Check KNIM... | Ballit... Substructure search | 2012-10-05 08:36:... | 0.042 |

SiteMap and Run PyMOL nodes

- **SiteMap**
 - Identify potential binding sites.
 - Evaluate a single binding site region (using the parameter flow variables)

SiteMap Job control Flow Variables Memory Policy

Column containing input :

Require at least site points per reported site

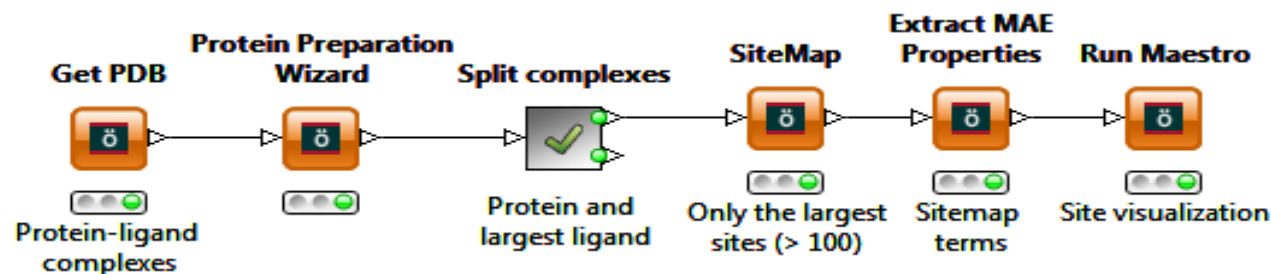
Report up to sites (site-point groupings)

Use definition of hydrophobicity

Use grid

Crop site maps at Å from nearest site point

☐ Keep log files



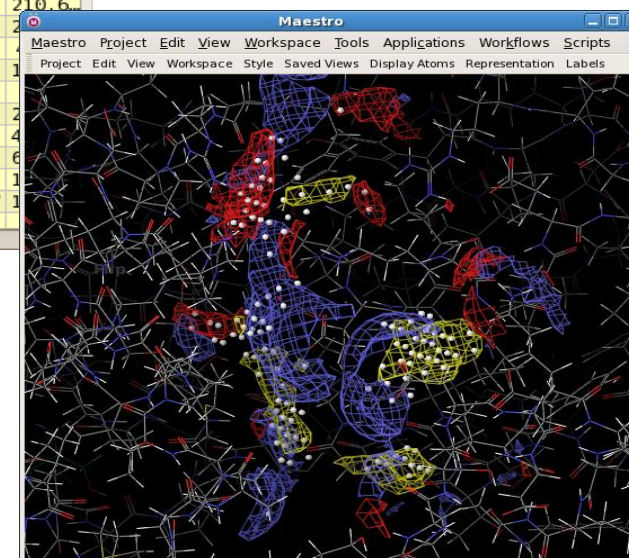
| Row | Stars | In | Title | Entry ID | SiteScore | size | Dscore | volume |
|------|-------|-------------------------------------|---------------------|----------|-----------|------|--------|----------|
| [12] | | | [1] - internal_M... | | | | | |
| 1 | ☆☆☆☆ | <input checked="" type="checkbox"/> | 1YTK_site_1 | S | 1.027 | 125 | 1.067 | 385.8... |
| 2 | ☆☆☆☆ | <input type="checkbox"/> | 1YTK_site_2 | S | 0.966 | 81 | 0.723 | 210.6... |
| 3 | ☆☆☆☆ | <input type="checkbox"/> | 1YTK_site_3 | S | 0.956 | 73 | 1.001 | |
| 4 | ☆☆☆☆ | <input type="checkbox"/> | 1YTK_site_4 | S | 0.806 | 21 | 0.723 | |
| 5 | ☆☆☆☆ | <input type="checkbox"/> | 1YTK_site_5 | S | 0.772 | 56 | 0.774 | |
| 6 | ☆☆☆☆ | <input checked="" type="checkbox"/> | 1YTK | | | | | |
| 7 | ☆☆☆☆ | <input type="checkbox"/> | 3DT1_site_1 | S | 1.169 | 125 | 1.238 | 2... |
| 8 | ☆☆☆☆ | <input type="checkbox"/> | 3DT1_site_2 | S | 1.020 | 150 | 0.951 | 4... |
| 9 | ☆☆☆☆ | <input type="checkbox"/> | 3DT1_site_3 | S | 0.958 | 230 | 0.989 | 6... |
| 10 | ☆☆☆☆ | <input type="checkbox"/> | 3DT1_site_4 | S | 0.773 | 56 | 0.718 | 1... |
| 11 | ☆☆☆☆ | <input type="checkbox"/> | 3DT1_site_5 | S | 0.683 | 34 | 0.637 | 1... |
| 12 | ☆☆☆☆ | <input type="checkbox"/> | 3DT1 | | | | | |

PyMOL Flow Variables Memory Policy

Column containing input :

PyMOL location:

Command Script:



Standard input/output and Glide ligand docking node

- More nodes **input and output pdb and sdf**.

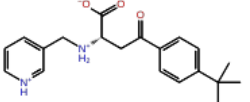
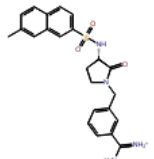
No need of converters.

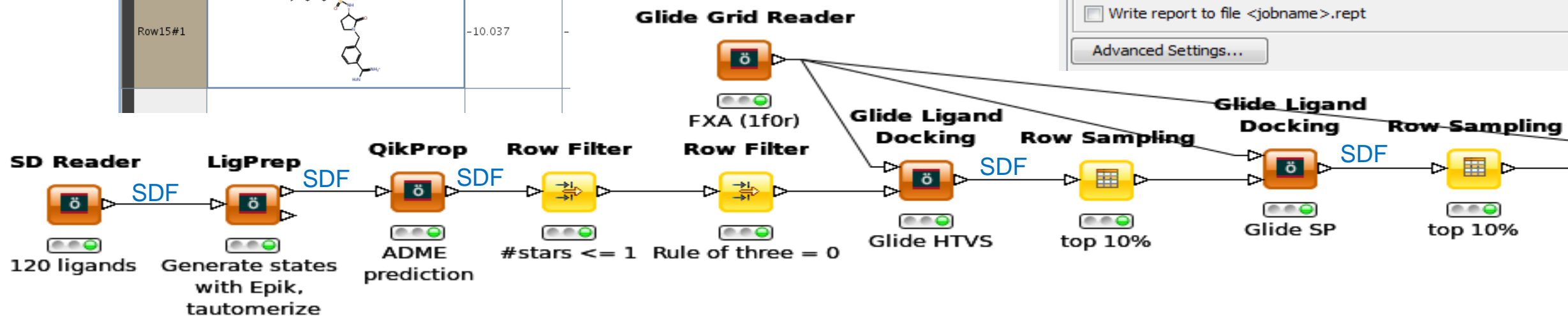
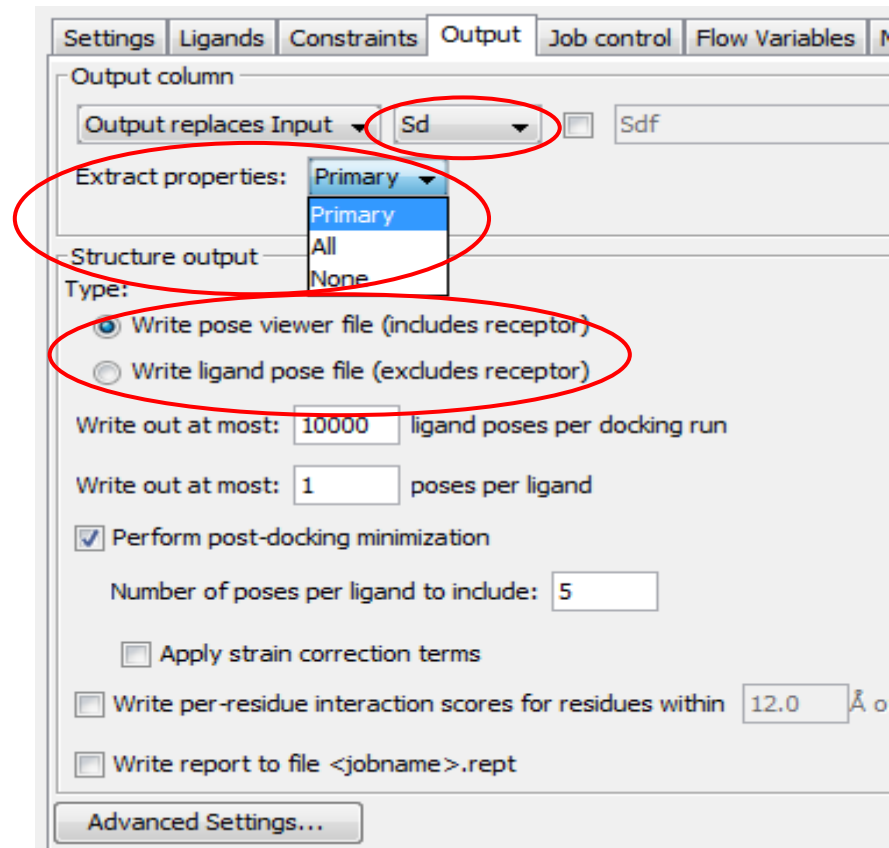
Glide ligand docking, Run Maestro command, Assign bond order, Split by Structure...

- Extract automatically** the generated properties

Prime MM-GBSA and Glide ligand docking

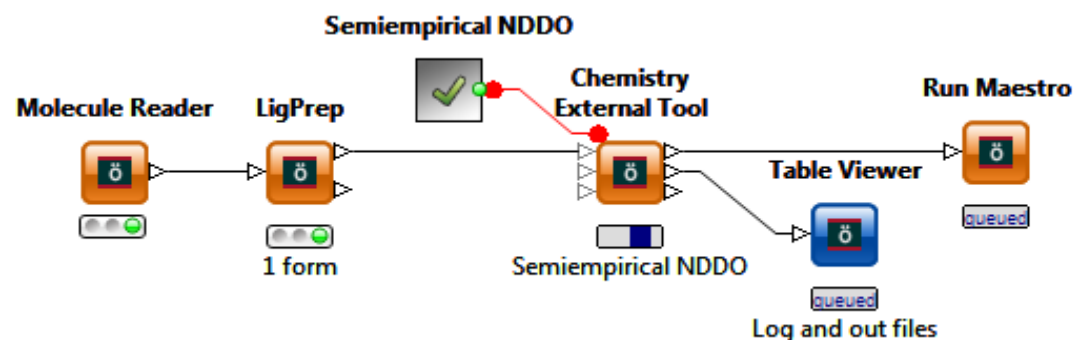
- Glide ligand docking** with 1 output

| Row ID | SDF Sdf | Docking score |
|---------|--|---------------|
| Row47#4 |  | -8.233 |
| Row15#1 |  | -10.037 |



New Chemistry external tool node

- **Optional input/output ports**, output column structure options, column name.
- Reads maegz files, input/output pdb, output Surface type
- **Flow variables, accessible by name**
- **Basename keyword, add extra columns** to the output



Quickforms Job Manager Selection

Method:

- ☒ RM1
- ☐ PM3
- ☐ AM1
- ☐ MNDO
- ☐ MNDOd

Optimize geometry ☒

Keywords: esp mullik bonds pi super plotesp

Host: localhost

ChemExternalTool Flow Variables Memory Policy

Input columns

Input1 (%input_1%): CT

Input2 (%input_2%):

Input3 (%input_3%):

☐ Run command line for each input row

Output replaces Input Maestro ☐ CT

Output only Text ☒ log

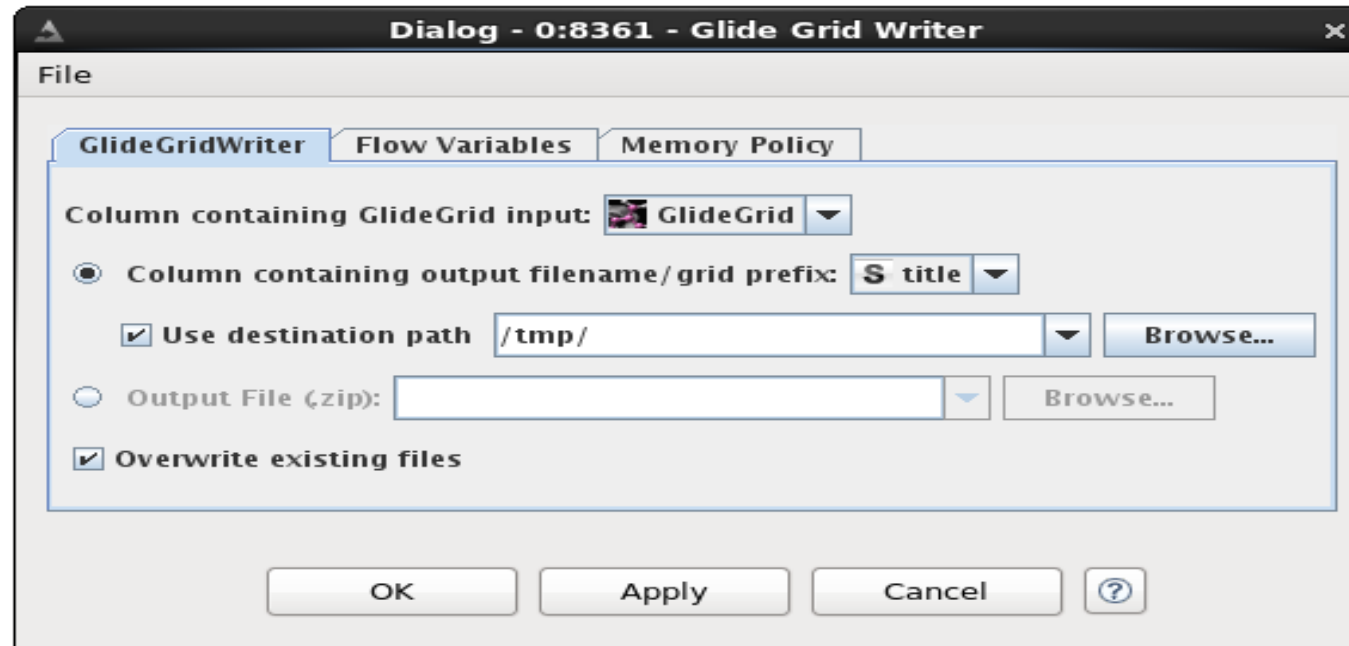
Output replaces Input Maestro ☐ CT

Command line(s):

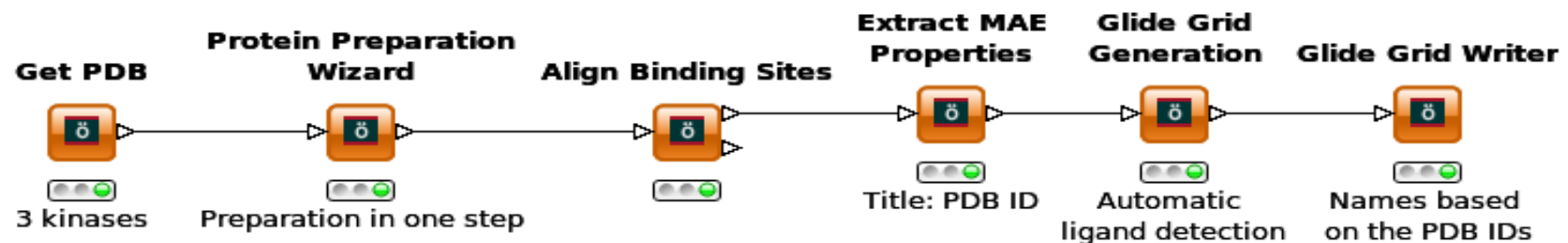
```
$SCHRODINGER/run semi_emp.py -WAIT -HOST %HOST% %Options% -jobname %basename_1% %input_1%  
mv %basename_1%.out.mae %output_1%  
cat %basename_1%.log %basename_1%_1.out %basename_1%_2.out > %output_2%
```


Glide grid writer

- Output file name + increment or from a column



- See Docking > Grid generation 1-3 workflow example



Webservice

- In the LigPrep node:

~/schrodinger/schrodinger.hosts:

name: pdx_web_server

host: pdx-bld-l02.schrodinger.com

port: 8080

processors: 3

- Called from the Generic Webservice Client node

For various tools with 1 input and 1 output

eg LigPrep, QikProp

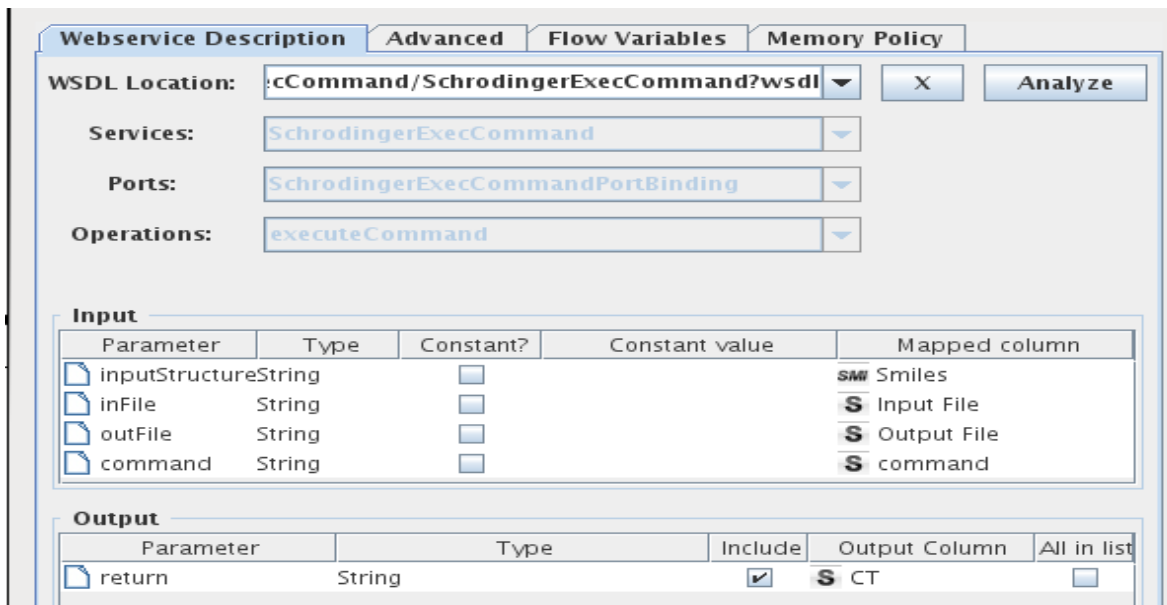
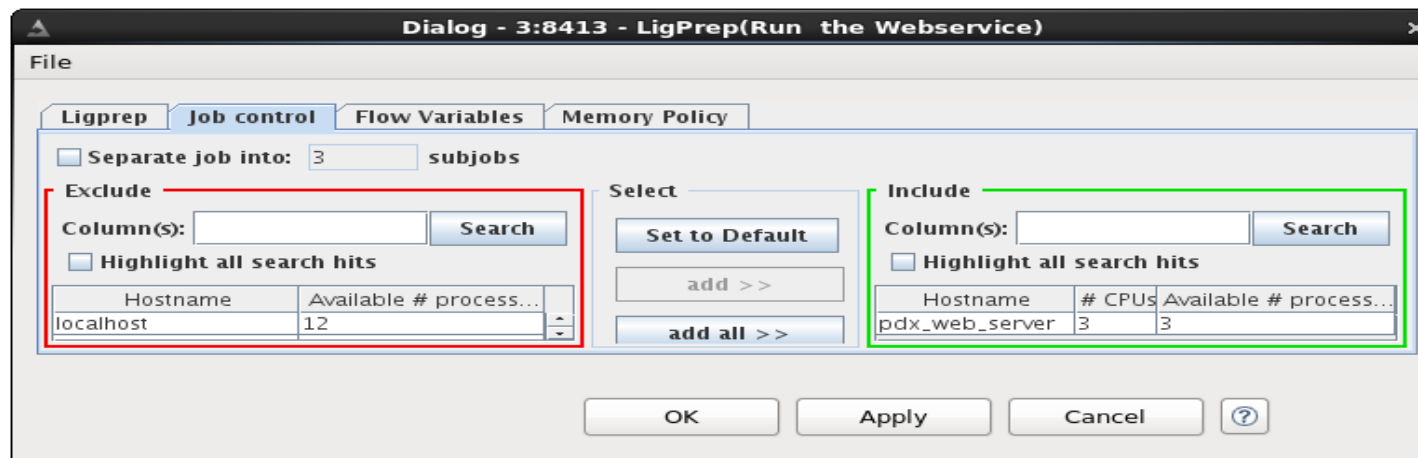
SCHRODINGER/ligprep -WAIT -HOST localhost:1

-nz -nc -s 4 -r 1 -epik -i 2 -W 'e,-ph,7.0,-pht,2.0'

-ismi ligprep_in.smi -osd ligprep_out.sdf

See General tools > Webservice

workflow example



2013-1 new features

Based on KNIME 2.7

Infrastructure improvements

- Environment for a stand-alone installation configurable in the preferences.
Set-up diagnosis node.
- Generation of the command line to be run in batch based on node annotations, batch execution setting panel. So workflows can easily be run in Seurat
- Parameter flow variables to use any backend command line option not exposed in the node configuration panel
- Workflow examples available in the installation

New nodes

- SiteMap
- Run PyMOL
- Workflow list – lists the nodes and workflows in the workspace

New functionalities

- KNIME in Maestro – input structures from files
- More nodes input and output pdb and sdf
eg Glide ligand docking, Assign bond order, Split by Structure
- Prime MM-GBSA and Glide ligand docking – Extract automatically the generated properties
- Parameter flow variable – Glide ligand docking, Prime nodes, Protein preparation wizard, SiteMap, some Jaguar, MacroModel and Canvas nodes.
- Glide ligand docking – with 1 output, sdf output type and other new functionalities
- Chemistry external tool – with optional input/output ports, access to the flow variables by name, basename and other new keywords.
- And many other fixes and minor improvements

2013-2 and 2013-3 New Features

2013-2

- Latest version of KNIME (v2.8.2), included in 2013-3
- Glide Grid Generation node- Save options
- Glide Multiple Grid Reader- Columns indicating original file location
- Run Maestro- Optionally provide command line arguments

2013-3

- Easily specify custom configuration at application start
- Restored cross-platform 2D renderer functionality in the embedded KNIME installation
- Can invoke **web service** to execute LigPrep node
- Execute some Schrödinger backends through the Generic Web Service Client node
- New **Glide grid writer** node
- Flow variables can be used in the run Maestro command node script
- Expanded reporting from the Setup diagnosis node

2012 New Features – Infrastructure and Usability

Infrastructure

- Based on KNIME 2.5.1
- Ported to **Mac OS X**
- **Start-up script** improvements including options to use a stand-alone KNIME installation, specify the KNIME temporary directory.

On Windows the bat window is silenced.

Usability

- The backend options reported in the console for all our nodes
- License checking mechanism improved to speed up the KNIME start-up
- Some nodes no longer require a Schrödinger KNIME license:

Reader, Writer, Converter, Scripting, KNIME-Maestro Connector, Run Maestro, and Canvas

KNIME 2.5 – some New Features

- **Node annotation** - multiline, copy/paste, select all. Custom description via context menu
- Align nodes vertically
- **Table view** - select and copy a block of cells, sort data by clicking the column header (2 levels)

New functionalities and nodes

- **String Manipulation** node - for operations on string columns
- JFreeChart nodes - new image output port (to be used in reports)
- **Database nodes** – new functionalities (schema browser, multi-line SELECT and non-SELECT queries)

Still not straightforward to update a database

KNIME 2.4- some New Features

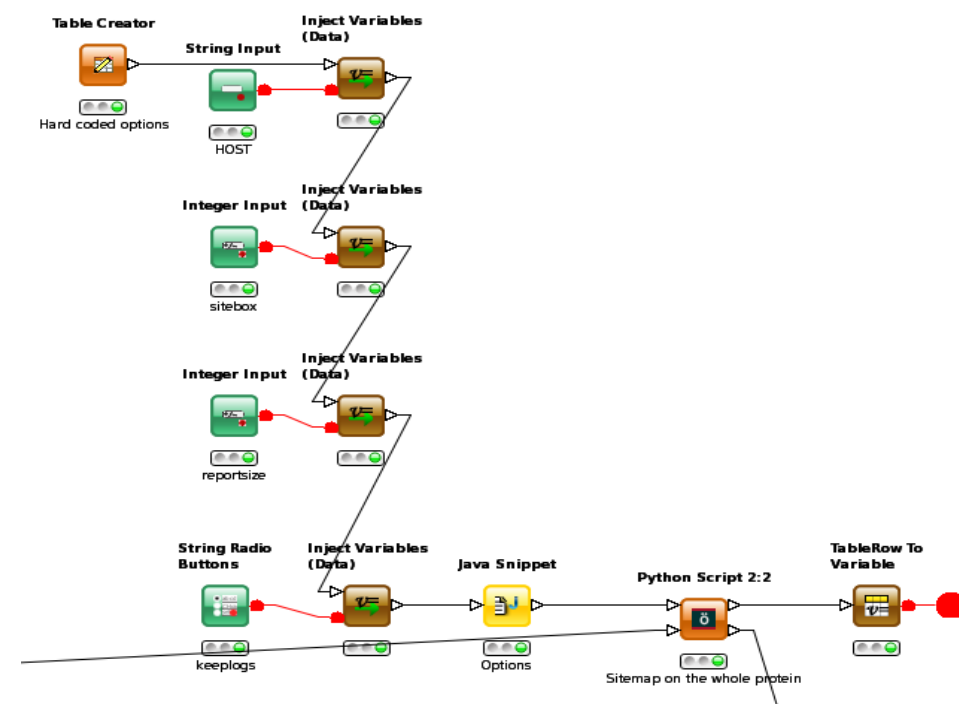
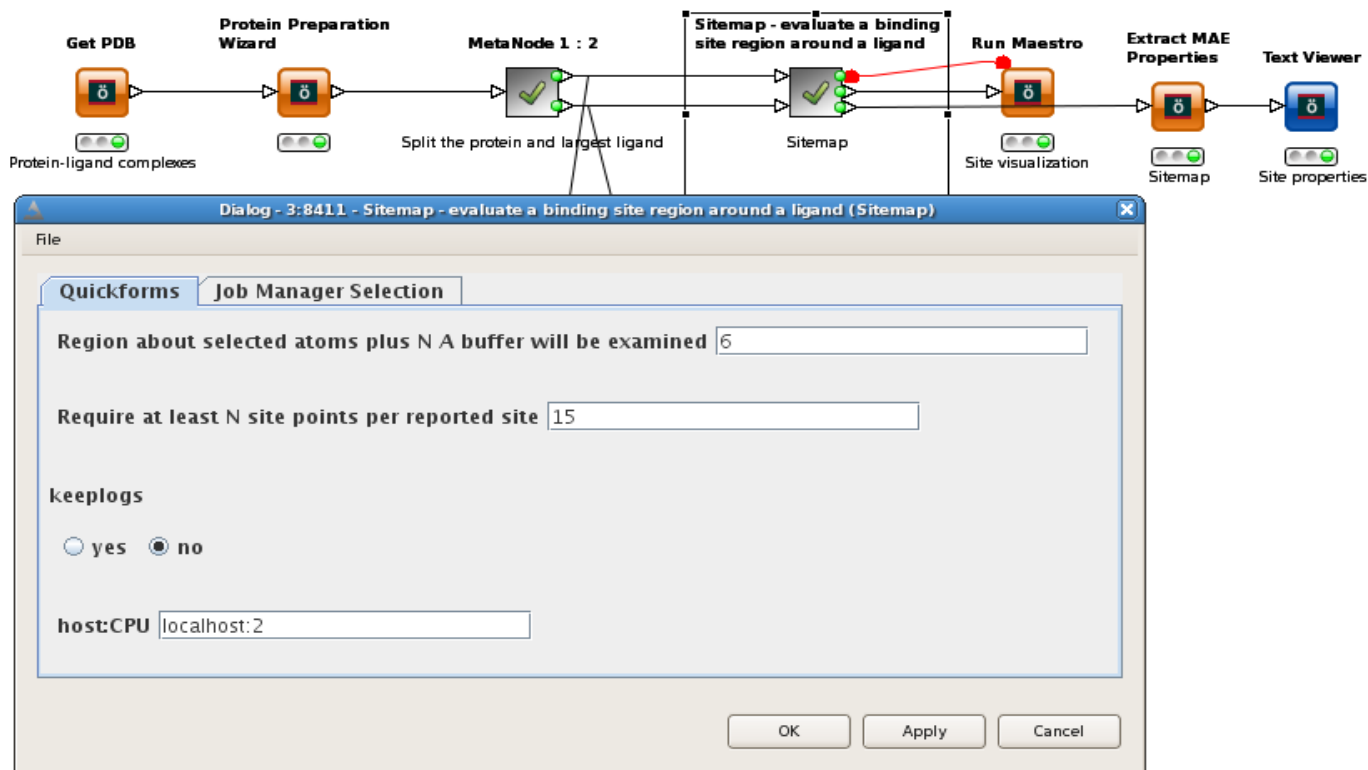
- **Meta node** - collapse, expand, rename
- **Quick form** node settings on a workflow or meta node level
- **Auto-layout** (experimental), fast node insertion
- Looping execution - step, pause, **parallel execution**. Column list loop start
- **Shorter start-up time** (nodes loaded on demand, batch execution)

New functionality and nodes:

- **Free Marvin nodes**
- **XML processing nodes**
- **SDF Reader** - multiple files, limit rows... CSVReader and Writer - handle gzipped files. Line reader.
- **GroupBy**- new aggregation methods. **Pivoting** - more aggregation methods and multiple group and pivoting columns. Column to grid – group.
- **Insert column header**, Column Rename (Regex), Equal Size Sampling, Line Reader, Create Temp Dir, Binner (Dictionary), Write PNG Image, Crosstab (contingency table)

Metanode with Quick Form Based Configuration Panel

- The new Quick form nodes in KNIME 2.4 make possible to create a new “node” with a configuration dialog without requiring Java programming
- This is actually a metanode exposing some configuration settings that can be passed to a Python script node as in the example below



Start-up Script - Options

Only affects the current session (don't permanently alter the workspace settings in KNIME preferences)

- **-help** .. Print information on command line options
- **-data <directory>** ... Use <directory> as the KNIME workspace rather than the default of ~/workspace
- **-maxHeap <value>** ... Set maximum heap size to <value>
ex: -maxHeap 1024m
- **-maxThreads <value>** ... Set maximum working threads to <value>
- **-defaultHost <value>** ... Set default host from the schrodinger.hosts file (default is localhost)
- **-deleteTempFiles <value>** ... Set option to delete temporary files (true or false)
- **-ooCmd <value>** ... Set Open Office Spreadsheet command to <value>
- **-schrodingerTempDir <directory>** ... Set Schrodinger temporary directory to <directory>.

If <directory> is "FromSchrodingerHost", then the value of 'tmpdir:' for 'localhost' in schrodinger.hosts file will be used.

- **-knimeTempDir <directory>** ... Set KNIME temporary directory to <directory>.

If <directory> is "FromSchrodingerHost", then the value of 'tmpdir:' for 'localhost' in

schrodinger.hosts file will be used.

- **-knimeInstallDir <directory>** ... Set the KNIME installation directory to <directory>.

It can also be specified in the schrodinger.hosts file adding a line knime: <path> in the localhost section. This installation is then used in the Maestro workflows menu.

Batch execution specific options:

- **-batch** ... Invoke the batch executor/engine
- **-nosave** ... Do not save the workflow after execution has finished
- **-reset** ... Reset workflow prior to execution
- **-preferences** ... path to the file containing eclipse/knime preferences
- **-workflowFile=<file> or -workflowDir=<dir>** ... Workflow as zip or in a workspace
- **-destFile=<file.zip> or -destDir=<dir>** ... Place where the executed workflow should be written (otherwise only saved in place)
- **-option=nodeID,name,value,type** ... Set the option with name 'name' of the node with ID 'nodeID' to the given 'value', which has type 'type'
- And a couple others (see the -help message)

Start-up Script - Applications

- Human readable option names (eg batch, memory)
 - Instead of `knime -Xmx4096m` or in `knime.ini`
- Define the Schrodinger environment and use the start-up script options with a stand alone installation (`-knimeInstallDir`), shell silenced on Windows
- Use several KNIME versions, extensions in beta test (`-knimeInstallDir`)
- Easy file clean up (`-knimeTempDir` and `-schrodingerTempDir`)
- Use a workspace on different machines (`-maxHeap` `-schrodingerTempDir` `-knimeTempDir` `-maxThreads`) and platforms (`-ooCmd` `-defaultHost`)
- Make sure you didn't forget to turn on Delete temporary files again (`-deleteTempFiles true`)
- Example:

```
knime -maxHeap 4096m -max_threads 5 -defaultHost localhost  
-schrodingerTempDir /tmp/KNIME/ -knimeTempDir /tmp/  
-deleteTempFiles true -ooCmd oocalc -data mainKNIMEworkspace/
```

KNIME menu in Maestro under workflows

Structure exchange

- To send structures to and from an open KNIME session

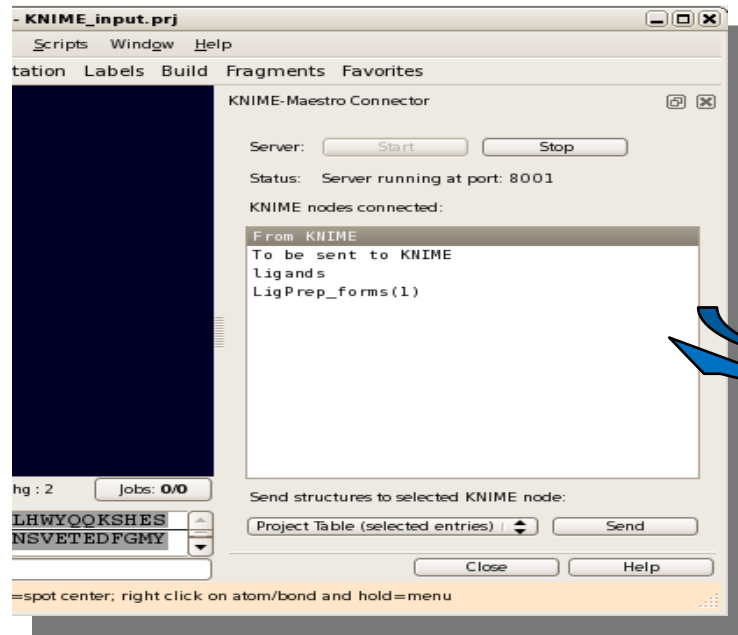
Run KNIME workflows

- Build, import, edit and run workflows from Maestro on project table data.
Input, output from Maestro specified by changing node names.
Dynamically generated GUI to alter some parameters.
- Rename and organize workflows in categories.
They can also be installed under Scripts (running a workflow doesn't required any knowledge about KNIME)
- Disconnected calculations and progress tracking in Jobcontrol
- Workflow tools and examples available on the Workflow web page:
 - Process PDB codes, Split and align multimers, Binding site RMSD matrix
 - Nearest neighbour similarity distribution, Substructure search
 - others will be added to the workflow page (eg Compound set filtering)

KNIME – Maestro connection

Maestro

Visual inspection, selections ...



Project table

Store the results

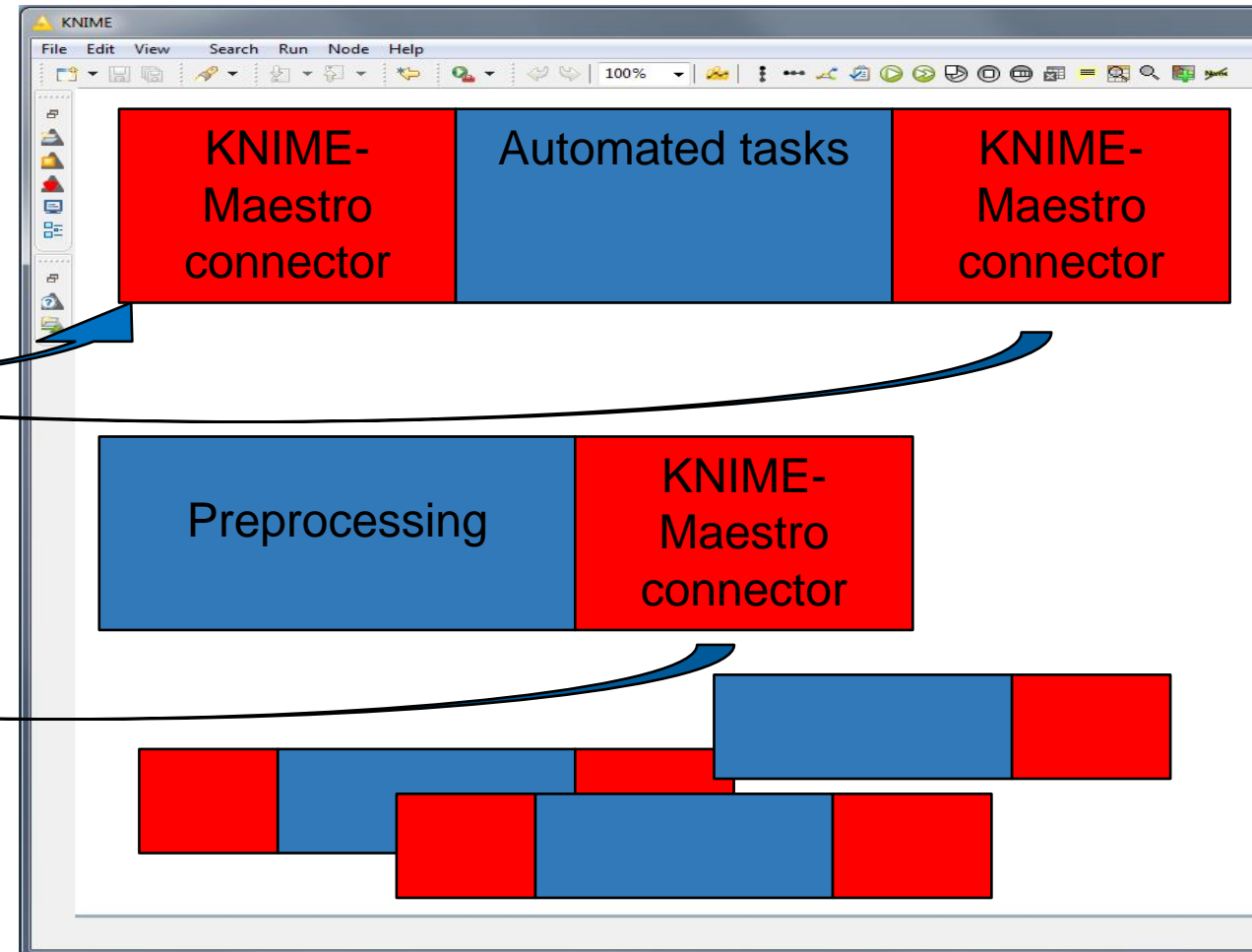
The screenshot shows the 'Project Table' window with a table of docking results. The table has columns for Row, Stars, In, Title, and docking score.

| Row | Stars | In | Title | docking score |
|------|-------|----|----------------------------------|---------------|
| [3] | | - | [1] - Crystal structures | |
| 1 | ☆☆☆☆ | ☐ | 1AC8 | |
| 2 | ☆☆☆☆ | ☐ | 1AET | |
| 3 | ☆☆☆☆ | ☐ | 1AC4 | |
| [8] | | + | [2] - Known active | |
| [17] | | + | [3] - Inactive compounds | |
| [54] | | + | [4] - Ligprep forms | |
| [55] | | - | [5] - MaestroCmd_34402818517213_ | |

Server

KNIME

used interactively



Maestro - KNIME structure exchange

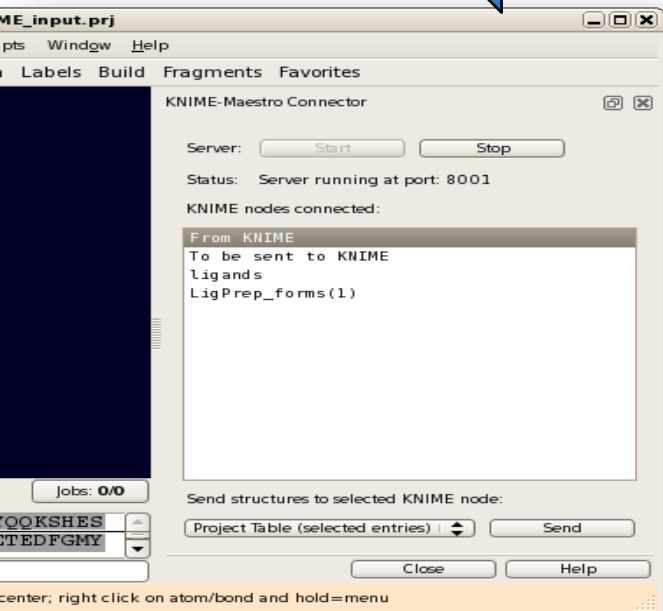
Maestro

Server

KNIME

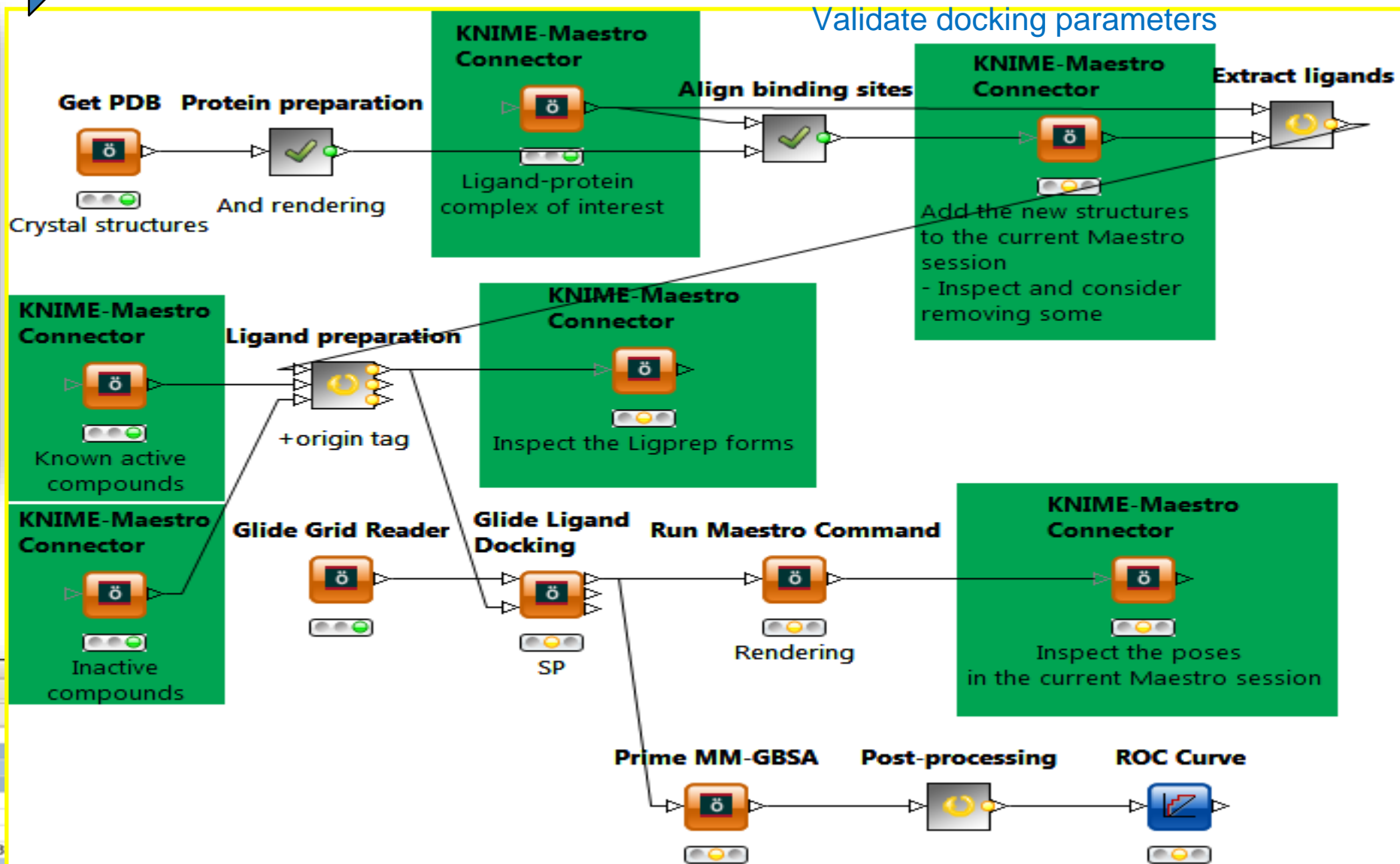
<http://www.schrodinger.com/knimeworkflows/>

Validate docking parameters



Project table

| Row | Stars | In | Title |
|------|-------|----|---------------------------------|
| [3] | | - | [1] - Crystal structures |
| 1 | ☆☆☆☆ | ☐ | 1AC8 |
| 2 | ☆☆☆☆ | ☐ | 1AET |
| 3 | ☆☆☆☆ | ☐ | 1AC4 |
| [8] | | + | [2] - Known active |
| [17] | | + | [3] - Inactive compounds |
| [54] | | + | [4] - Ligprep forms |
| [55] | | - | [5] - MaestroCmd_34402818517213 |



Run workflows from Maestro

The screenshot displays the Maestro - KNIME_input.prj application window. The 'Workflows' menu is open, showing options like 'Protein Preparation Wizard...', 'Virtual Screening Workflow...', and 'P450 Site of Metabolism'. The main workspace shows a 3D molecular model of a protein-ligand complex. The right panel is titled 'PDB list preparation' and contains the following configuration:

- Input:** None
- Output:**
 - New group
 - Maestro message Warning if the structures are prepared automatically
- Parameter:**
 - PDB code list - PDB codes: 1W84, 1W83, 1W7H, 1OUY
 - PDB code list - Mode: Preprocess

At the bottom, there are 'Run', 'Cancel', and 'Help' buttons. The status bar at the bottom left shows 'Jobs: 0/0', 'Atoms: 0/3511/5720', 'Entries: 1/1900', 'Res: 363', 'Chn: 1', 'Mol: 12', and 'Chg: -9'.

Run workflows from Maestro

The image displays two software windows: Maestro and KNIME, illustrating the integration of workflows.

Maestro - KNIME_input.prj

- Menu: **Workflows**
- Sub-menu: **KNIME**
- Options: Protein Preparation Wizard..., Virtual Screening Workflow..., Induced Fit Docking..., QM-Polarized Ligand Docking..., Ligand and Structure-Based Descriptors..., P450 Site of Metabolism

PDB list preparation

Load a list of PDB codes and preprocess or prepare them automatically.

Open in KNIME... (highlighted with a red circle) **Create a Copy**

Input: None

Output:

- New group
- Maestro message Warning if the structures are prepared automatically

Parameter: (highlighted with a red circle)

PDB code list - PDB codes: 1W84, 1W83, 1W7H, 1OUY

PDB code list - Mode: Preprocess

☐ Save after execution

Run **Cancel** **Help**

KNIME

File Edit View Node Search Run Help

*0: PDB_list_preparation *0:25 - PDB code list

String Radio Buttons

Java Edit Variable

String Input

Get PDB

Mode GUIsettingCOMBO (highlighted with a red circle) **Switch**

PDB codes GUIsetting

Run workflows from Maestro

The image displays the Maestro - KNIME_input.prj application window. The 'Workflows' menu is open, showing options like 'Protein Preparation Wizard...', 'Virtual Screening Workflow...', and 'P450 Site of Metabolism'. Below the menu, a 'Monitor' window shows a table of job execution details. The 'PDB list preparation' workflow configuration panel is also visible, showing input, output, and parameter settings.

Maestro - KNIME_input.prj

Maestro Project Edit View Workspace Tools Applications Workflows Scripts Window Help

Connect to KNIME...
New...
Manage...
Install...
Update...
Install examples
Vendor database filtering...
Cheminformatics
Filtering
General tools

KNIME

- Protein Preparation Wizard...
- Virtual Screening Workflow...
- Induced Fit Docking...
- QM-Polarized Ligand Docking...
- Ligand and Structure-Based Descriptors...
- P450 Site of Metabolism

Monitor

| Job ID | Name | Status | Errs | Start Time | Host | Application | Project |
|-------------------------|------------------------|----------------------|------|---------------------|--------------|---------------|-----------------|
| workstation2-0-4edfla01 | Vendor_database_fil... | incorporated : fi... | 0 | 2011-12-07-08:47:12 | workstation2 | KNIME | KNIME_input.prj |
| workstation2-0-4edfla51 | MolecularDescripto... | completed | 0 | 2011-12-07-08:48:33 | workstation2 | KNIME | KNIME_input.prj |
| workstation2-0-4edfla58 | MolecularDescripto... | completed | 0 | 2011-12-07-08:48:40 | workstation2 | KNIME | KNIME_input.prj |
| workstation2-0-4edfla5e | MolecularDescripto... | completed | 0 | 2011-12-07-08:48:46 | workstation2 | KNIME | KNIME_input.prj |
| workstation2-0-4edfla65 | MolecularDescripto... | completed | 0 | 2011-12-07-08:48:53 | workstation2 | KNIME | KNIME_input.prj |
| workstation2-0-4edfla6b | MolecularDescripto... | completed | 0 | 2011-12-07-08:48:59 | workstation2 | KNIME | KNIME_input.prj |
| workstation2-0-4edfla96 | Ligprep_in_3751460... | completed : finis... | 0 | 2011-12-07-08:49:42 | workstation2 | Para_LigPr... | KNIME_input.prj |
| workstation2-1-4edfla99 | Ligprep_in_375146... | completed : finis... | 0 | 2011-12-07-08:49:45 | workstation2 | Ligprep | KNIME_input.prj |
| workstation2-0-4edfla9c | Ligprep_in_375146... | completed | 0 | 2011-12-07-08:49:48 | workstation2 | Ligprep | KNIME_input.prj |
| workstation2-0-4edfla9e | Ligprep_in_375146... | completed | 0 | 2011-12-07-08:49:50 | workstation2 | Ligprep | KNIME_input.prj |
| workstation2-0-4edfla9f | Ligprep_in_375146... | completed | 0 | 2011-12-07-08:49:51 | workstation2 | Ligprep | KNIME_input.prj |
| workstation2-0-4edfla99 | PDB_list_preparatio... | completed : finis... | 0 | 2011-12-07-08:49:45 | workstation2 | KNIME | KNIME_input.prj |
| workstation2-0-4edflaab | prepwizard_lgxxl_i... | completed | 0 | 2011-12-07-08:50:03 | workstation2 | ProtAssign | KNIME_input.prj |
| workstation2-0-4edflab6 | prepwizard_lgxxl_i... | completed | 0 | 2011-12-07-08:50:14 | workstation2 | ProtAssign | KNIME_input.prj |

Show: [Jobs from this project only] Monitor frequency: 1 sec
Monitor Pause Resume Stop Kill Update Delete... Clean Up Postmortem... Refresh

Details File

File: /home/jc/Projects/current/PDB_list_preparation_pIUC9zbiF14k.log

Running KNIME in batch...
DEBUG Workflow: /home/jc/.schrodinger/maestro93/workflows/PDB_list_preparation_dir/PDB_list_preparation
STATUS Running KNIME: /usr/local/schro-latest/maestro93/workflows/PDB_list_preparation_dir/PDB_list_preparation -nosave -
option=39,output_file_name,/tmp/PDB_list_preparation_pIUC9zbiF14k_l_new_group.mae,String "-option=25/21,value/value,1W84, 1W83,String" -
option=25/22,value/value,Preprocess,String

Finished in 28 secs (28369ms)

STATUS : finished command line

PDB list preparation

Load a list of PDB codes and preprocess or prepare them automatically.

Open in KNIME... Create a Copy

Input:
None

Output:
- New group
- Maestro message Warning if the structures are prepared automatically

Parameter:
PDB code list - PDB codes 1W84, 1W83, 1W7H, 1OUY
PDB code list - Mode: Preprocess

☐ Save after execution

Run Cancel Help

Splits and align multimers

Run from Maestro

Maestro

Maestro Project Edit View Workspace Tools Applications Workflows Scripts Window Help

Project Edit View Workspace Style Saved Views Display Atoms Representation Labels Build Fragments Favorites

Title: 1CX2
PDB ID: 1CX2

Split and align multimers

Split protein multimers by chain ID and align binding sites.

Open in KNIME... Create a Copy

Input:

- Selected entries (homomultimers)

Output:

- New group - in the project table

Parameter:

Align: ☒ Yes ☐ No

☐ Save after execution

Run Cancel Help

String Radio Buttons Java Edit Variable

Molecule Reader

Split

Assign bond order and Split by structure

String Radio Buttons

Alignment or not GUIsettingRADIO

Java Edit Variable

IF Switch

Alignment or not

Protein alignment

End IF

Molecule Writer

New group - in the project table

2D Show 2D Structure Show Family

| Row | Stars | In | Title | Entry ID | Entry Name | PDB TIT | PDB ID | PDB RESOLU | PI |
|-----|-------|----|------------------------------|----------|----------------------------|----------|--------|------------|----|
| [2] | | | [1] - Process_PDB_codes_f... | | | | | | |
| 1 | ☆☆☆☆ | ■ | 1CX2 | 1 | Process_PDB_codes_ft82L... | CYCLO... | 1CX2 | 3.000 | X- |
| 2 | ☆☆☆☆ | □ | 1SO2 | 2 | Process_PDB_codes_ft82L... | CATAL... | 1SO2 | 2.400 | X- |

2012 New Features – Functionalities

Functionalities

- Phase shape - ability to search a database
- New **surface column type** – created with the Python script node and displayed with Run Maestro node
- Phase hypothesis and Glide grid types- display and access to the path
- **Python script node new functions** and access to the flow variables

Many fixes and minor improvements

- Some nodes were renamed (eg Table Viewer, Run Spreadsheet Viewer)

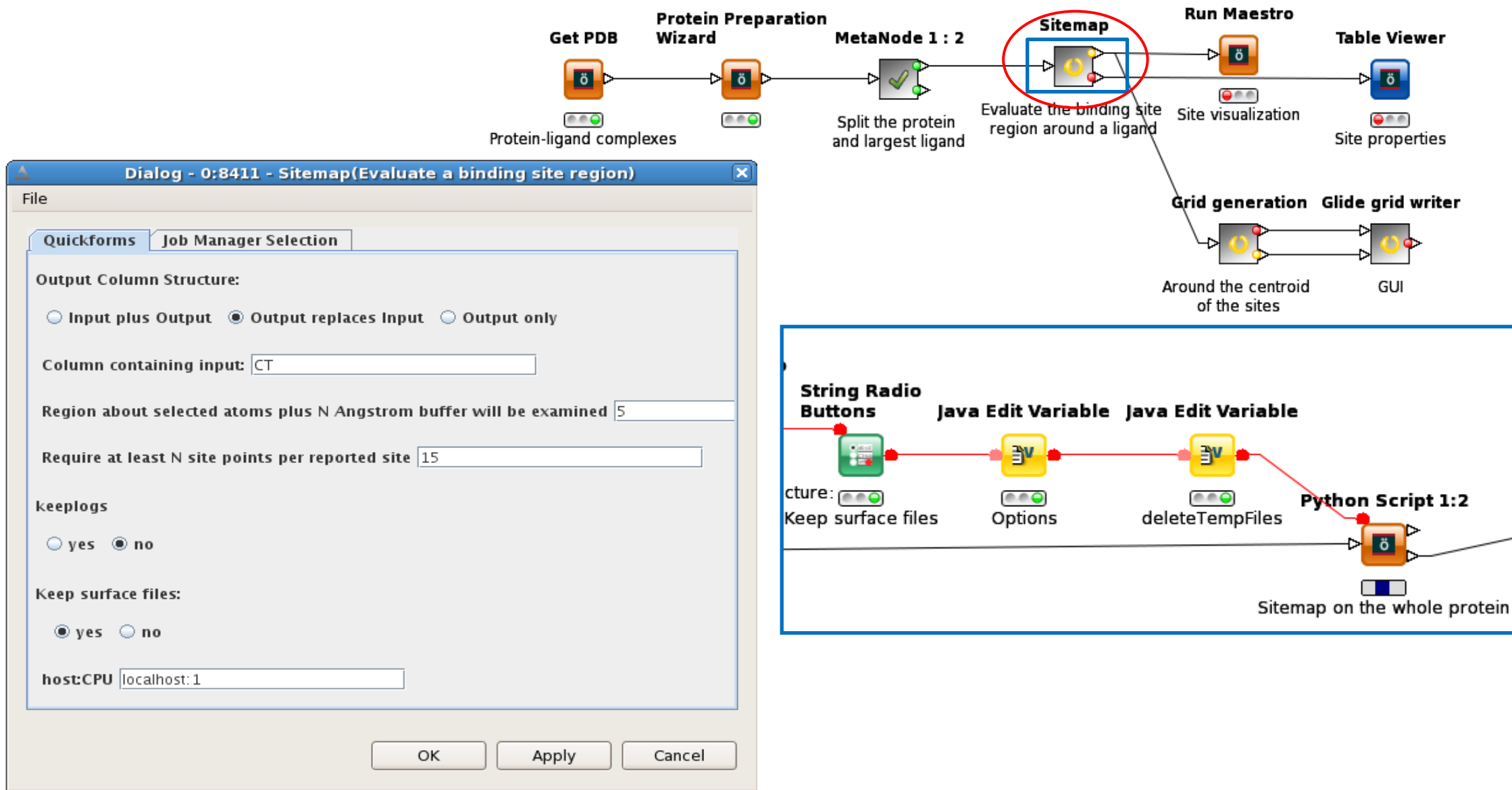
Metanodes (available on the Workflow page)

- **Run Maestro 1:1**
- **Run PyMOL**
- Jaguar pKa
- **Sitemap**
- Glide grid writer

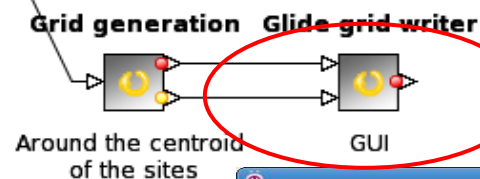
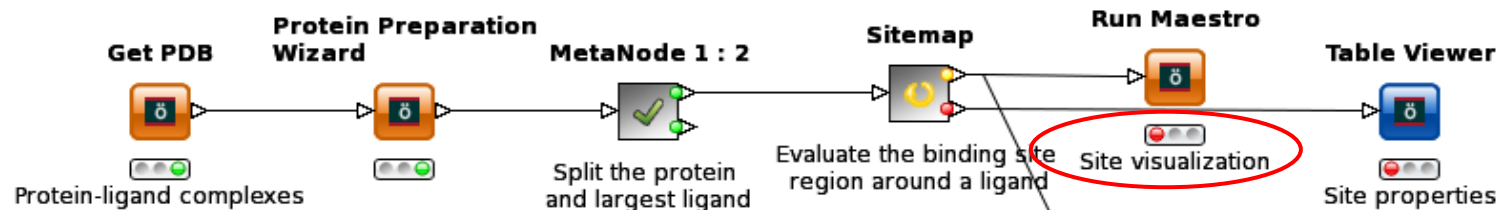
[List of all the nodes](#)

New workflow examples

Some new metanodes and surface cell type



Some new metanodes and surface cell type



Dialog - 0:8411 - Sitemap(Evaluate a binding site region)

File

Quickforms Job Manager Selection

Output Column Structure:

☐ Input plus Output ☒ Output replaces Input ☐ Output only

Column containing input: CT

Region about selected atoms plus N Angstrom buffer will be examined 5

Require at least N site points per reported site 15

keeplogs

☐ yes ☒ no

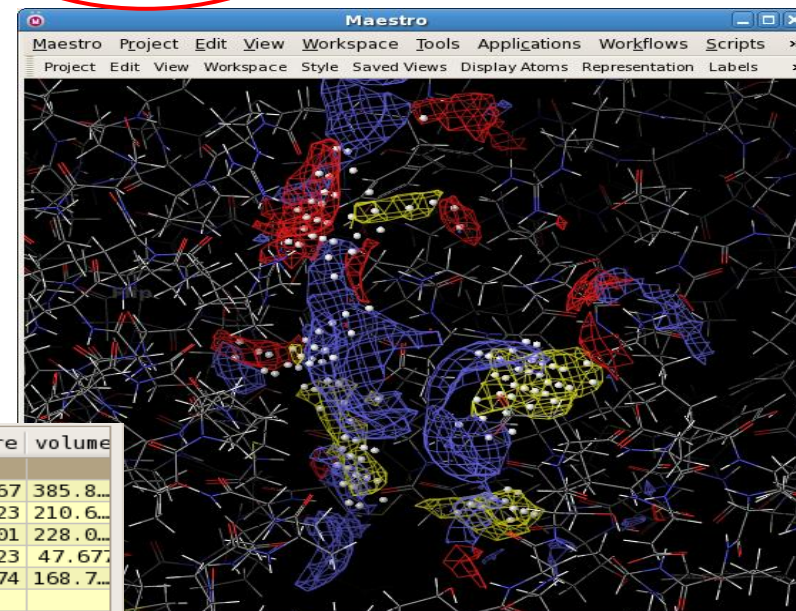
Keep surface files:

☒ yes ☐ no

host:CPU localhost:1

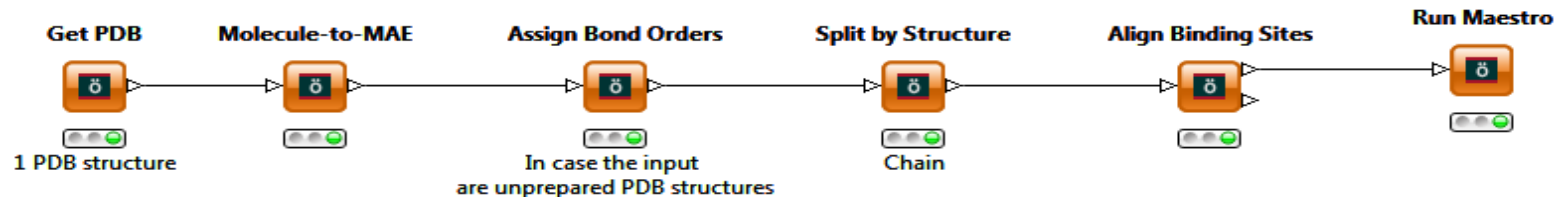
OK

| Row | Stars | In | Title | Entry ID | SiteScore | size | Dscore | volume |
|------|-------|----|---------------------|----------|-----------|------|--------|----------|
| [12] | | | [1] - internal_M... | | | | | |
| 1 | ☆☆☆☆ | ■ | 1YTK_site_1 | S 1 | 1.027 | 125 | 1.067 | 385.8... |
| 2 | ☆☆☆☆ | ■ | 1YTK_site_2 | S 2 | 0.966 | 81 | 0.723 | 210.6... |
| 3 | ☆☆☆☆ | ■ | 1YTK_site_3 | S 3 | 0.956 | 73 | 1.001 | 228.0... |
| 4 | ☆☆☆☆ | ■ | 1YTK_site_4 | S 4 | 0.806 | 21 | 0.723 | 47.67... |
| 5 | ☆☆☆☆ | ■ | 1YTK_site_5 | S 5 | 0.772 | 56 | 0.774 | 168.7... |
| 6 | ☆☆☆☆ | ■ | 1YTK | 6 | | | | |
| 7 | ☆☆☆☆ | ■ | 3DT1_site_1 | S 7 | 1.169 | 125 | 1.238 | 289.8... |
| 8 | ☆☆☆☆ | ■ | 3DT1_site_2 | S 8 | 1.020 | 150 | 0.951 | 468.1... |
| 9 | ☆☆☆☆ | ■ | 3DT1_site_3 | S 9 | 0.958 | 230 | 0.989 | 694.5... |
| 10 | ☆☆☆☆ | ■ | 3DT1_site_4 | S 10 | 0.773 | 56 | 0.718 | 110.7... |
| 11 | ☆☆☆☆ | ■ | 3DT1_site_5 | S 11 | 0.683 | 34 | 0.637 | 117.3... |
| 12 | ☆☆☆☆ | ■ | 3DT1 | 12 | | | | |

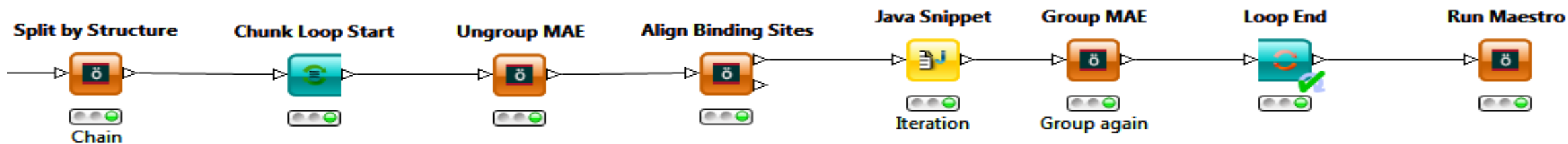


Splits and align multimers workflow example

Split a protein multimer by chain ID and align binding sites



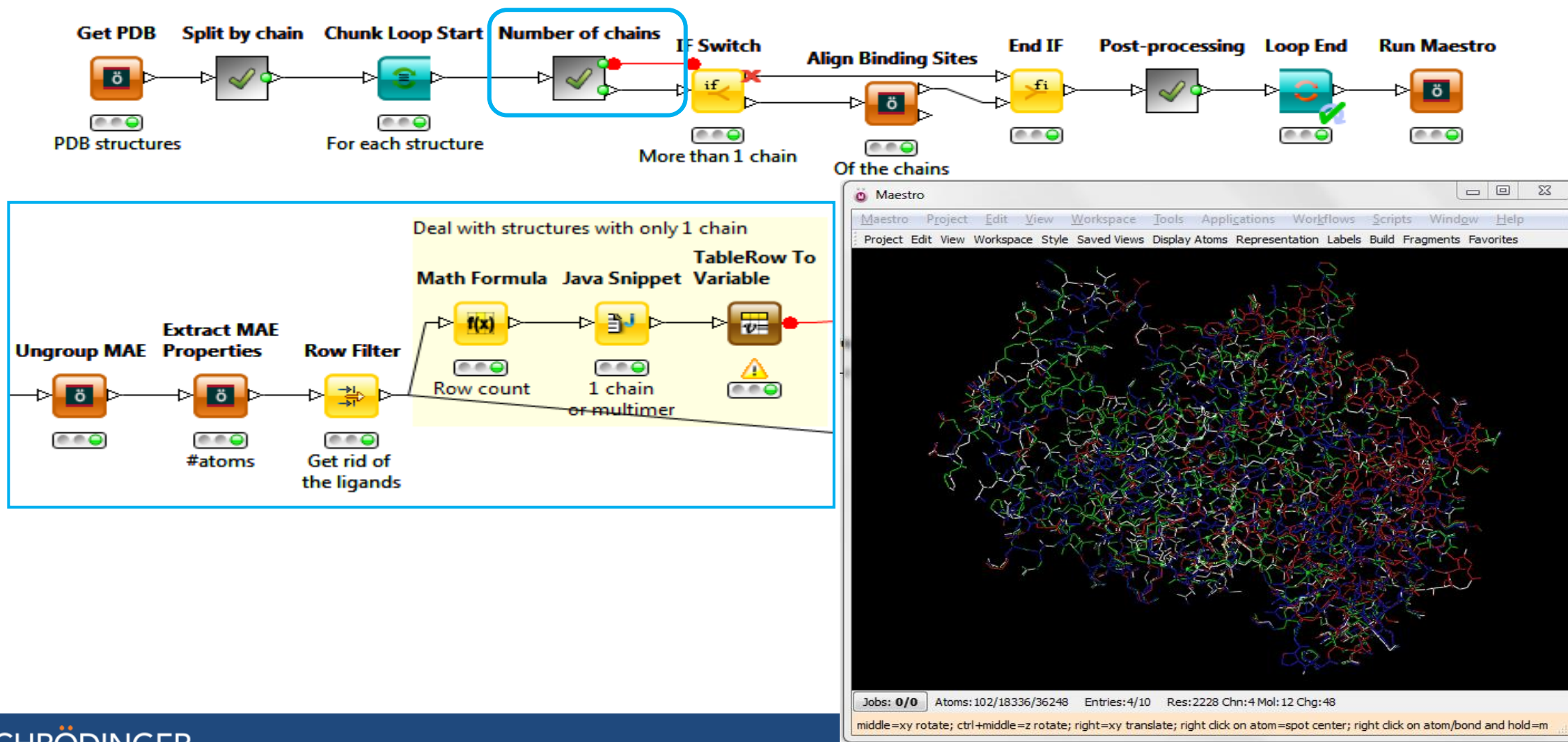
- Run on a set of multimers



| Row | Stars | In | Title | Entry ID | Entry Name | PDB Title | PDB ID | PDB |
|-----|-------|-------------------------------------|--------------------------------|----------|----------------------------|-----------|--------|-----|
| [2] | | | [1] - Process_PDB_codes_f... | | | | | |
| 1 | ☆☆☆☆ | <input type="checkbox"/> | 1CX2 | 1 | Process_PDB_codes_ft82L... | CYCLO... | 1CX2 | |
| 2 | ☆☆☆☆ | <input type="checkbox"/> | 1SO2 | 2 | Process_PDB_codes_ft82L... | CATAL... | 1SO2 | |
| [8] | | | [2] - Split_and_align_multi... | | | | | |
| 3 | ☆☆☆☆ | <input checked="" type="checkbox"/> | 1CX2 | 3 | Process_PDB_codes_ft82L... | CYCLO... | 1CX2 | |
| 4 | ☆☆☆☆ | <input checked="" type="checkbox"/> | 1CX2 | 4 | Process_PDB_codes_ft82L... | CYCLO... | 1CX2 | |
| 5 | ☆☆☆☆ | <input checked="" type="checkbox"/> | 1CX2 | 5 | Process_PDB_codes_ft82L... | CYCLO... | 1CX2 | |
| 6 | ☆☆☆☆ | <input checked="" type="checkbox"/> | 1CX2 | 6 | Process_PDB_codes_ft82L... | CYCLO... | 1CX2 | |
| 7 | ☆☆☆☆ | <input type="checkbox"/> | 1SO2 | 7 | Process_PDB_codes_ft82L... | CATAL... | 1SO2 | |
| 8 | ☆☆☆☆ | <input type="checkbox"/> | 1SO2 | 8 | Process_PDB_codes_ft82L... | CATAL... | 1SO2 | |
| 9 | ☆☆☆☆ | <input type="checkbox"/> | 1SO2 | 9 | Process_PDB_codes_ft82L... | CATAL... | 1SO2 | |
| 10 | ☆☆☆☆ | <input type="checkbox"/> | 1SO2 | 10 | Process_PDB_codes_ft82L... | CATAL... | 1SO2 | |

Splits and align multimers

Run on a set of structures (some of them may have only one chain)



Splits and align multimers

Run from Maestro

The image displays the Maestro software interface. The main window shows a 3D protein structure with four subunits colored grey, red, blue, and green. The title bar indicates 'Title: 1CX2' and 'PDB ID: 1CX2'. A 'Split and align multimers' dialog box is open on the right, with the following details:

- Input:** - Selected entries (homomultimers)
- Output:** - New group - in the project table
- Parameter:** Align: ☒ Yes, ☐ No
- ☐ Save after execution
- Buttons: Run, Cancel, Help

Below the main window, a workflow diagram is shown with the following steps:

- Molecule Reader** (Selected entries (homomultimers))
- Split** (Assign bond order and Split by structure)
- String Radio Buttons** (Alignment or not GUIsettingRADIO)
- Java Edit Variable**
- IF Switch** (Alignment or not)
- Protein alignment**
- End IF**
- Molecule Writer** (New group - in the project table)

At the bottom, a table lists the project entries:

| Row | Stars | In | Title | Entry ID | Entry Name | PDB TIT | PDB ID | PDB RESOLU' | P |
|-----|-------|----|------------------------------|----------|----------------------------|----------|--------|-------------|----|
| [2] | | | [1] - Process_PDB_codes_f... | | | | | | |
| 1 | ☆☆☆☆ | ■ | 1CX2 | 1 | Process_PDB_codes_ft82L... | CYCLO... | 1CX2 | 3.000 | X- |
| 2 | ☆☆☆☆ | □ | 1SO2 | 2 | Process_PDB_codes_ft82L... | CATAL... | 1SO2 | 2.400 | X- |

2011 New Features

Infrastructure

- **Windows** installers
- Canvas **2D renderer on 64 bit** KNIME workbench
- New **start-up scripts option**- memory limit, temporary directory... user/machine/OS-specific parameters

New nodes

- **Desmond** system builder and Molecular dynamics
- Desmond trajectory manipulation and extract frames
- Desmond trajectory and CMS Readers
- **Phase query on files** (already possible on a Phase database)
- **Canvas model** building and prediction nodes (PLS and Bayes classification)
- **Run Canvas**
- Filter structures based on an ASL expression
- Calculate properties

2011 New Features

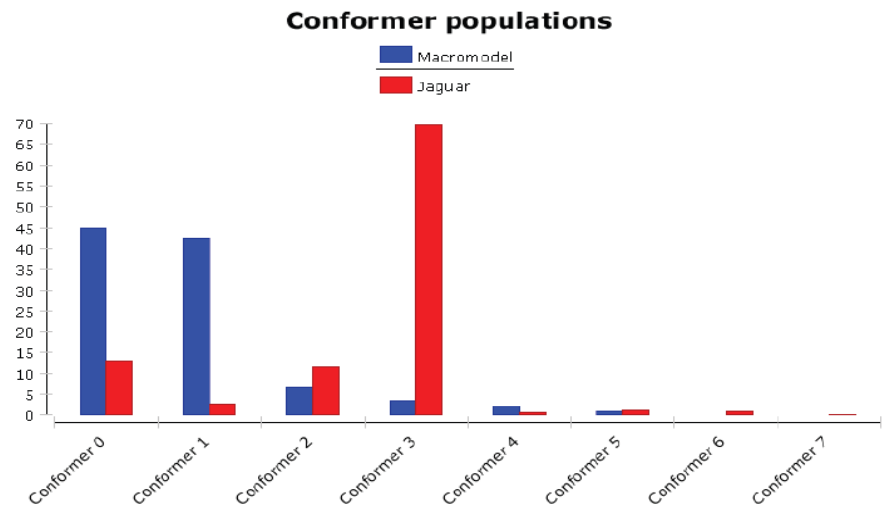
Node options and functionalities

- Prime Build homology model- include ligand and cofactors
- Run Maestro- import groups, read Hypotheses, specify a project to add the structures to
- Protein preparation wizard, Epik, Molecular descriptors- job distribution
- Ligprep- Implicit conversion

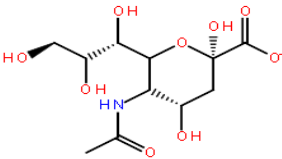
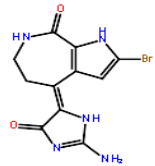
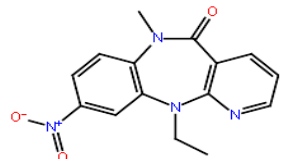
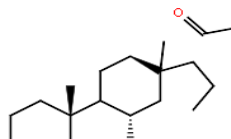
Even without a dedicated node

- Search PDB header, Ligand Interaction Diagram (using the Chem. ext. tool node)
- Variable based readers (flow variables port added to each node)
- Distance, angle or dihedral measurements (Python node)

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 |

| 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 |



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



KNIME 2.2- some new features

New features

- Add **flow variables port to each node**. Enables control on execution order
- Allow for **optional inputs**. See **Concatenate (Optional input)**
- **Loop-Concept for Chunking**- implement streaming like approach
see also Schrodinger Row iterator loop start node (one row at a time)
- Support for workflow-local files (separate storage in workflow folder)
- Preconfigured Workflow example server

New Nodes

- **Joiner** (more flexible matching criteria, scalability, composite keys,...)
- **Ungroup node**- Split Collection in Rows
- **Loop End node with two in/outputs**
- **CSV Reader** - more flexible than File Reader node when input structure changes
(Schrodinger's CSV reader node can read several files), **Excel reader** supports .xlsx
- In Labs: Web Analytics, **Spotfire nodes**, Modular Data Generation nodes
- Logistic Regression Learner & Applier, Item Set finder node ...

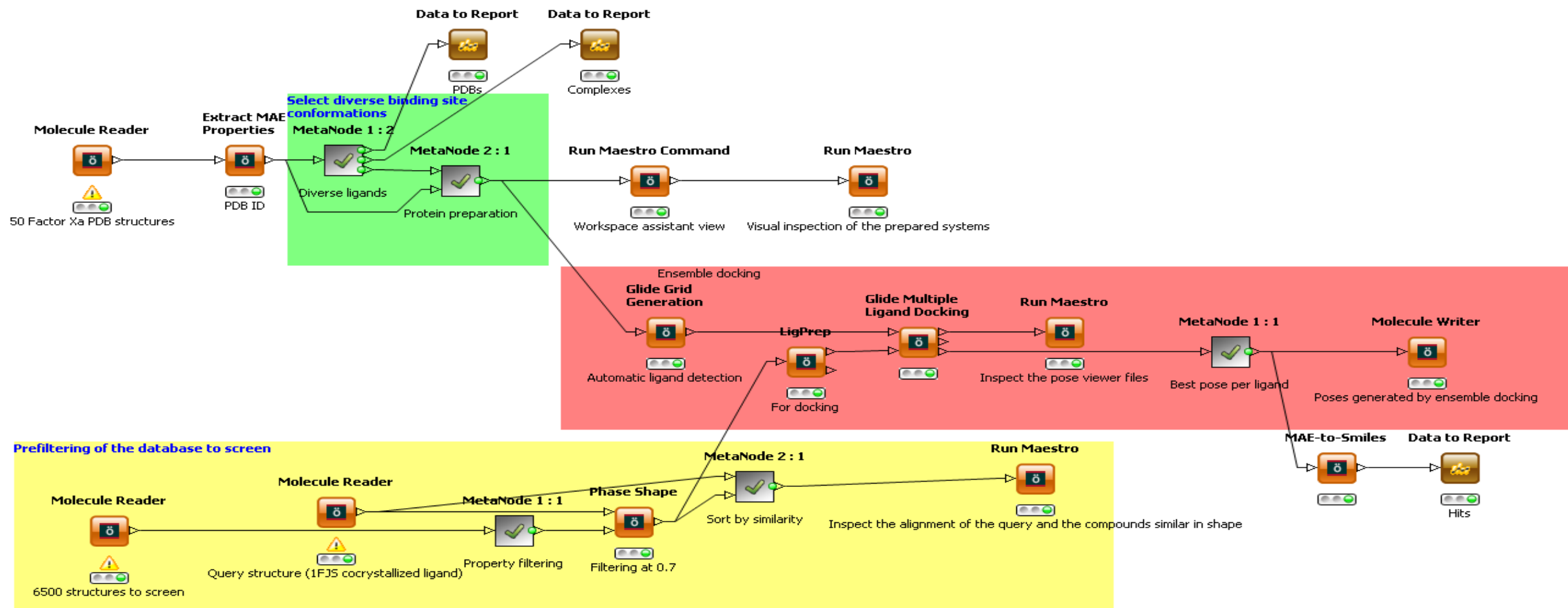
KNIME 2.3- some new features

- Upgrade to **Eclipse 3.6.1**/BIRT 2.6/Java 1.6.0_22: enables KNIME to fully run on Mac OS X, no more xulrunner version problem
- Sticky notes for **workflow annotation**
- Support for **Hotkeys** (e.g. to open a node's data output view)
- **Data Flow Switches**- IF/ENDIF, CASE/ENDCASE/ENDModelCASE nodes
- **Preference option to omit the default node label** ("Node 12") on node creation, to change the font size for node name and label. Switch to turn off the node labels above the nodes (e.g. "File Reader")
- **External tool**- can be used as **extension point** (Java code to create simple interfaces)
- Ability to export KNIME views and KNIME workflows as SVG image
- Boolean DataType, Variable support for Database Reader and Database Connector and "Image" port to carry, e.g. R views (needed for reporting)

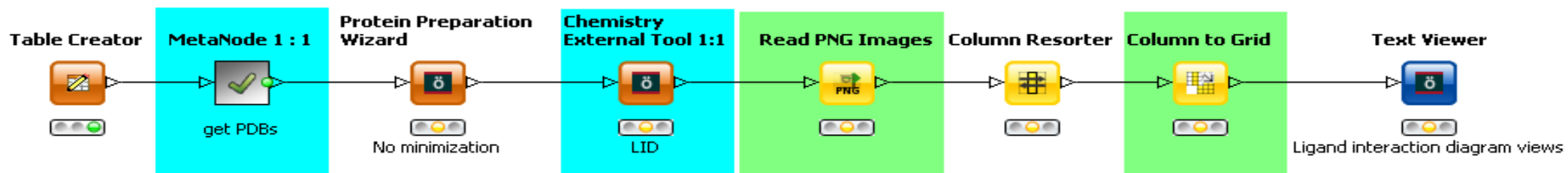
KNIME 2.3- some new nodes and functionalities

- **Table creator**- input the table content
Create Table Structure- empty table with predefined structure
- **Java Edit variable, Java Expression based Row Filter and Row Splitter**
- **Column to Grid**- split and turn a column to a grid to be used in a report table
- **Read PNG Images**, Image to Table and SVG Writer nodes
- **List Files**- list file locations
- **Loop End (Column Append)**- collecting columns instead of rows
- **Extract Column Header into data row**
- Excel Reader- speed improvements & user feedback on analyze
- A generic Cell replacer node
- Automatic Binner, Binner Apply nodes. Sparkline Appender node
- Java Snippet- Add Missing Value Handling, ability to throw exception (exits node execution)
- Variable support to be available in R nodes
- Extract System Properties (e.g. temp file, current user account)

Workflow annotations



Column to Grid, Read PNG images



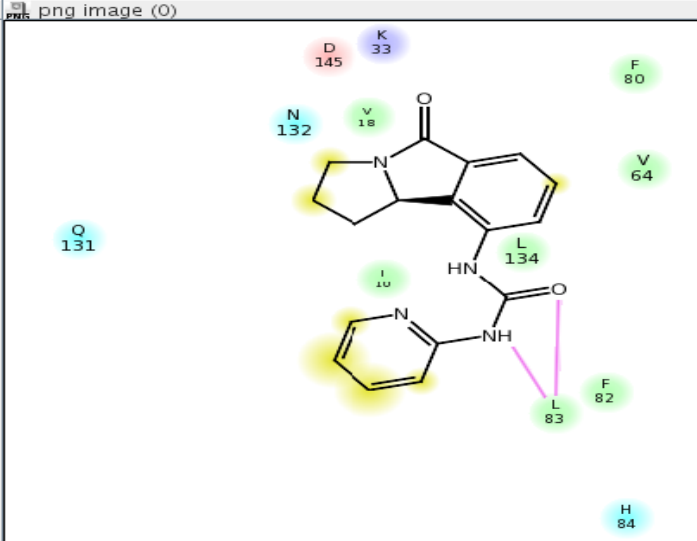
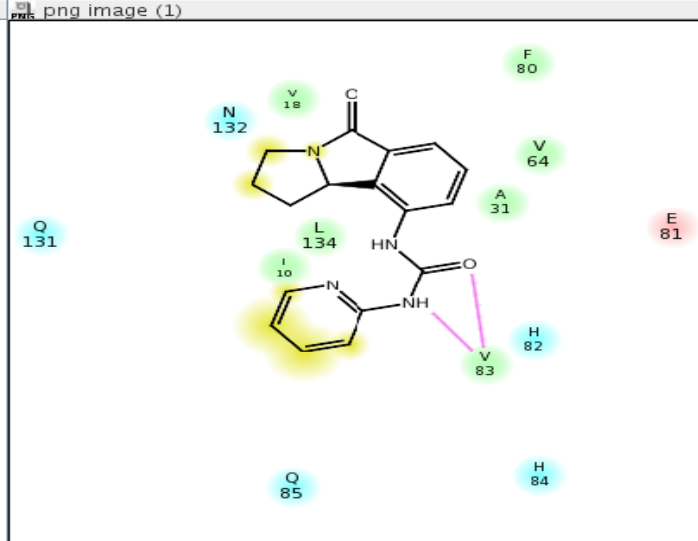
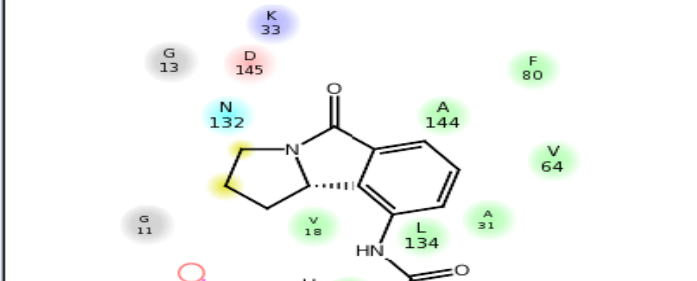
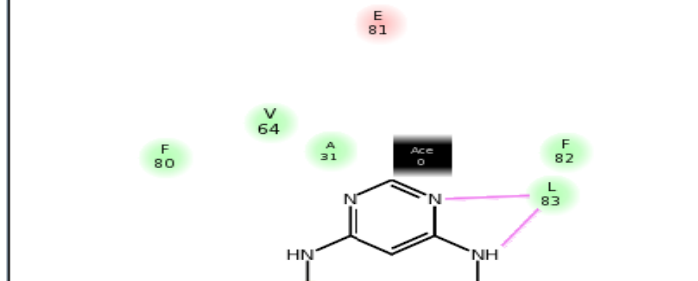
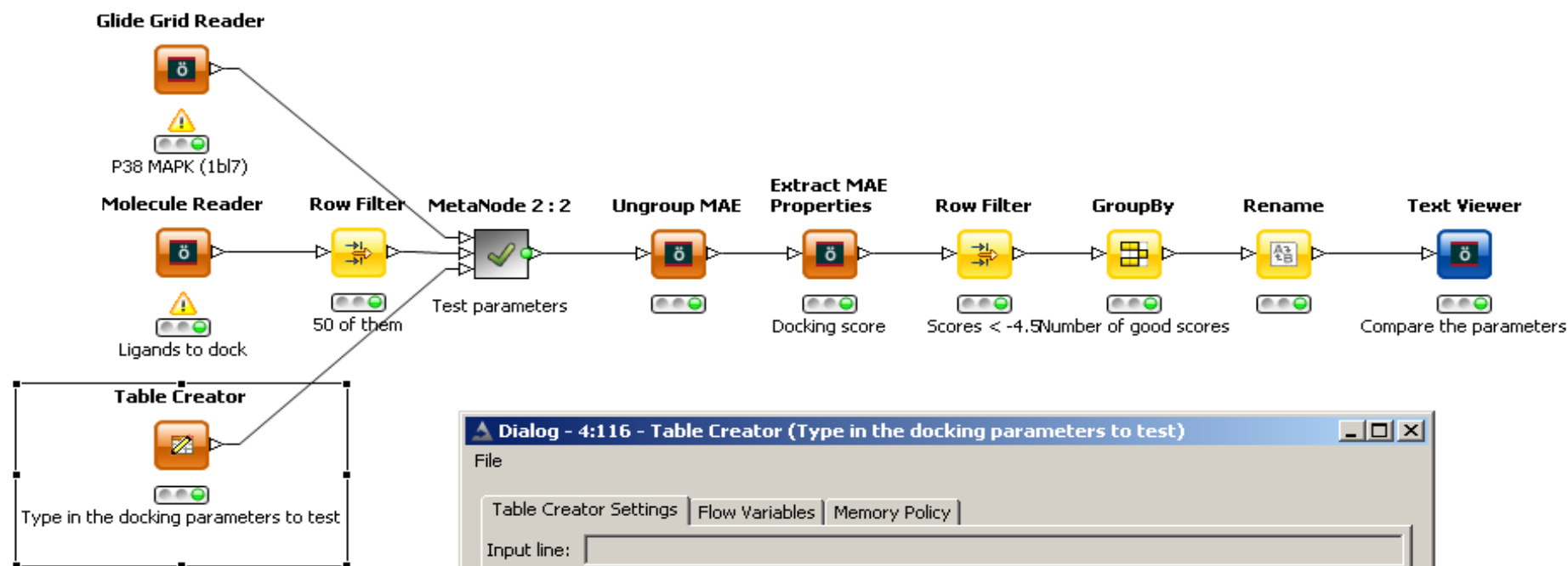
| Row ID | png image (0) | S ID (0) | png image (1) | S ID (1) |
|--------|--|----------|---|----------|
| Row0 |  | 1GIH |  | 1GII |
| Row1 |  | 1GIJ |  | 1H00 |

Table creator



Dialog - 4:116 - Table Creator (Type in the docking parameters to test)

File

Table Creator Settings | Flow Variables | Memory Policy

Input line:

| | S SP | S XP | S Epik | S Scale | | |
|------|-------------|-------------|---------------|----------------|--|--|
| Row1 | True | False | False | 0.8 | | |
| Row2 | True | False | True | 0.8 | | |
| Row3 | True | False | False | 1.0 | | |
| Row4 | False | True | True | 0.8 | | |
| Row5 | | | | | | |
| Row6 | | | | | | |
| Row7 | | | | | | |
| Row8 | | | | | | |

The output table has 4 rows and 4 columns. ☐ Highlight output table

OK Apply Cancel

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