

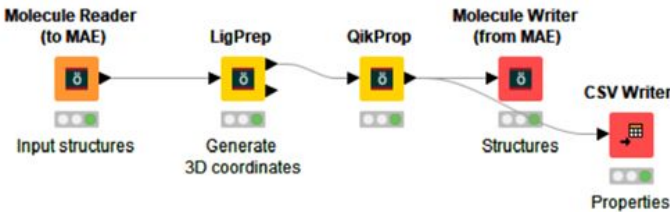
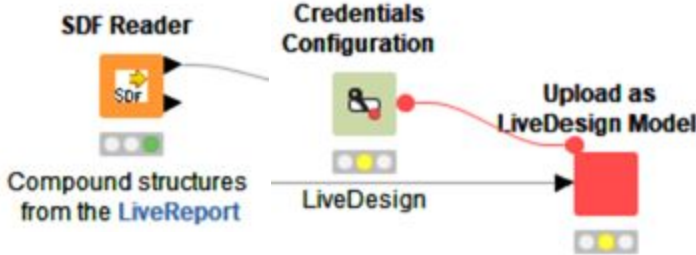
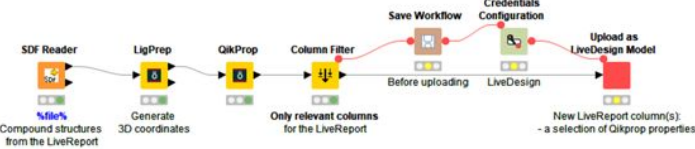
Turn a KNIME workflow into a computational model

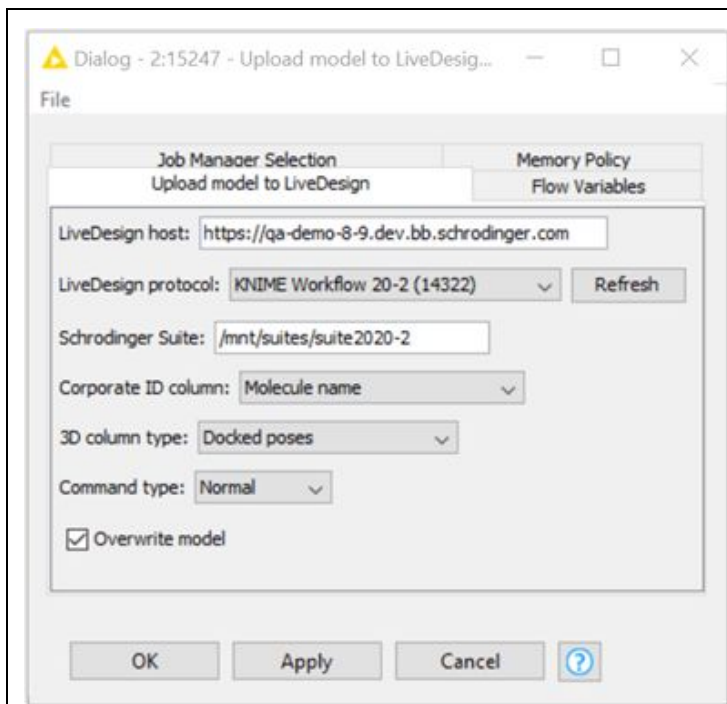
Created with: Release 8.9

Requirements: Schrödinger Suite 20-3 or newer installed locally and on the LiveDesign instance. A Live Report with compounds and properties.

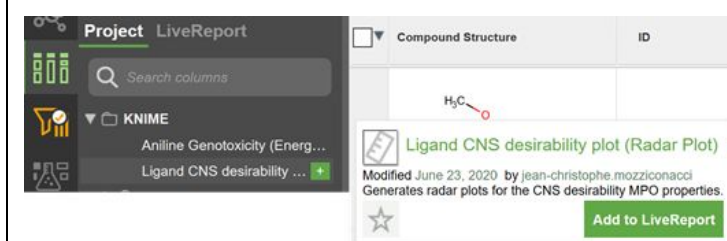
You can automate actions performed in Maestro with KNIME workflows and deploy them as models to LiveDesign.

- Some LiveDesign-ready workflows are available from:
https://hub.knime.com/schroedinger/spaces/LiveDesign_models/latest/
- Other KNIME workflow examples can be found in:
https://hub.knime.com/schroedinger/spaces/Workflow_examples/latest/

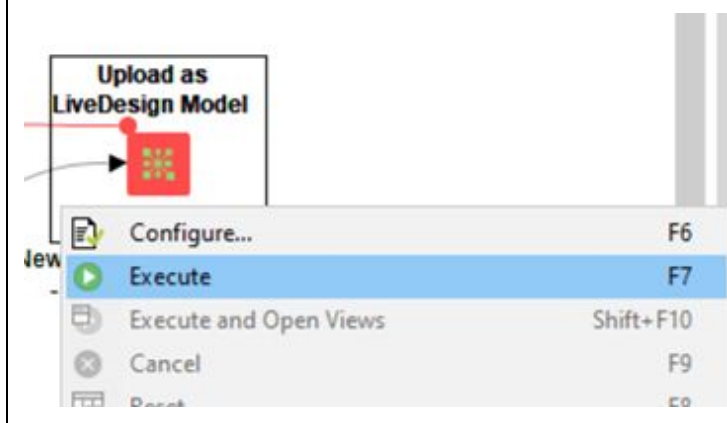
<p>\$SCHRODINGER/knime</p> 	<p>1. Open the workflow in KNIME.</p> <p>The example workflow has the following properties:</p> <ul style="list-style-type: none">• Input: 2D compound structures• Output: string, number columns and/or one 3D compound structure column. <p><i>Optional:</i> You can add any complex workflow in between input and output nodes</p> <p>If your KNIME workflow has different inputs or outputs, contact us for specific solutions.</p>
	<p>2. Use the SDF reader node as input</p> <p>3. Label it with “LiveReport”. It will read the structures from the LiveReport when the workflow is run in LiveDesign.</p> <p>4. Replace the output node(s) with the Upload model to LiveDesign node</p> <p>5. Add a Credential Configuration node.</p>
	<p>6. Save your workflow before configuring and executing the Upload node. It will create or update the corresponding LiveDesign model. The computational model is named after the KNIME workflow.</p>



7. Add your LiveDesign credentials to the **Credential Configuration** node.
8. **Configure the Upload** node with:
 - a. Your LiveDesign host address
 - b. Select the Protocol: in most of the scenarios you can use the generic KNIME Workflow protocol.
 - c. Select the column containing the Corporate ID
9. Execute the **Upload** node. The address of the computational model created/updated is printed in the KNIME console.



10. You can find the computational model under the **KNIME** folder in the **Computational model** section of your LiveDesign instance.



11. Changes to the workflow in KNIME can be deployed by re-executing the **Upload as LiveDesign** node again.