

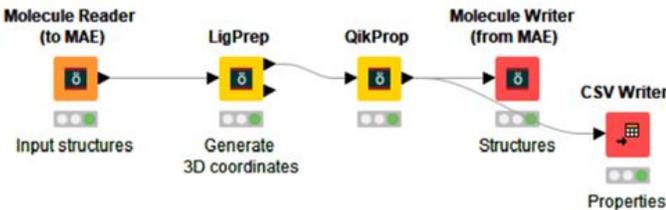
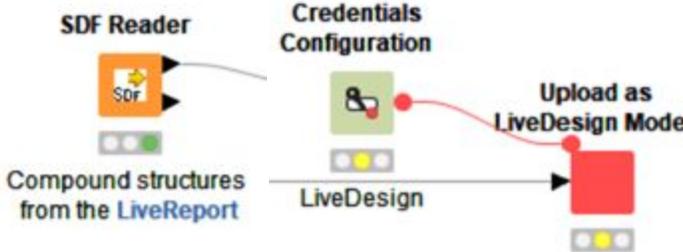
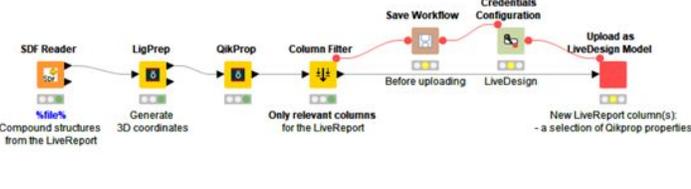
# Turn a KNIME workflow into a computational model

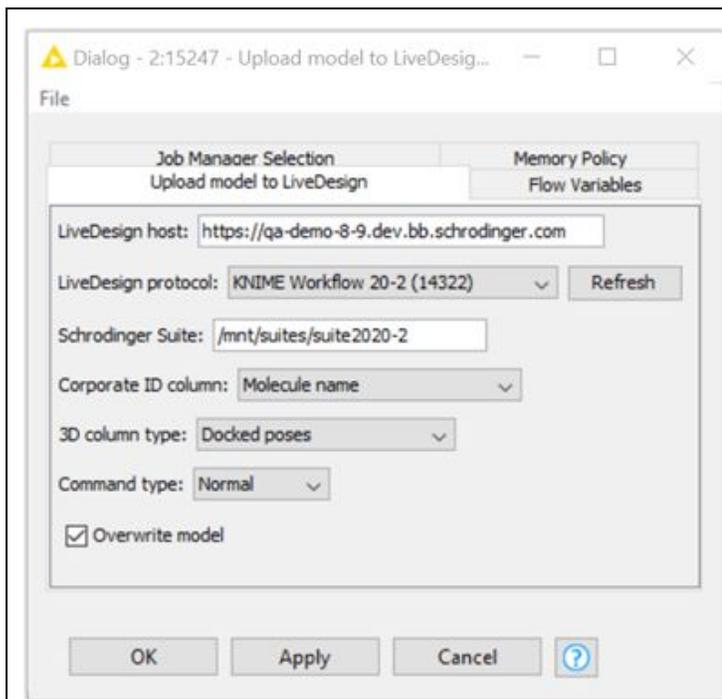
**Created with:** Release 8.9

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

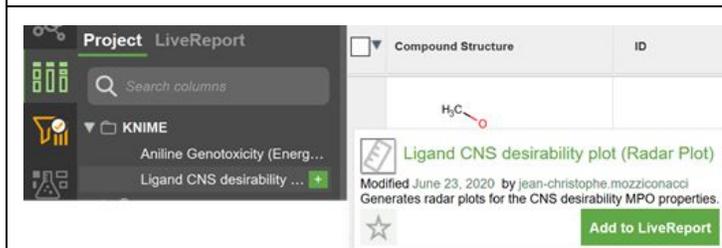
You can automate actions performed in Maestro with KNIME workflows and deploy them as models to LiveDesign.

- Some LiveDesign-ready workflows are available from: [https://hub.knime.com/schroedinger/spaces/LiveDesign\\_models/latest/](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/](https://hub.knime.com/schroedinger/spaces/Workflow_examples/latest/)

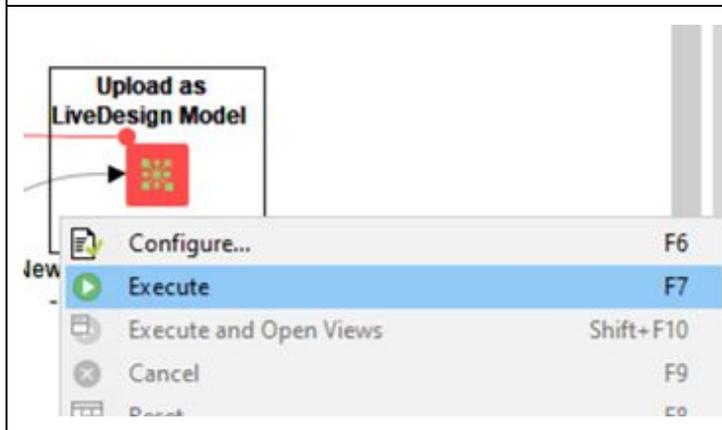
<p>\$SCHRODINGER/knime</p>  <p>The diagram shows a linear workflow: <b>Molecule Reader (to MAE)</b> (Input structures) → <b>LigPrep</b> (Generate 3D coordinates) → <b>QikProp</b> → <b>Molecule Writer (from MAE)</b> (Structures) → <b>CSV Writer</b> (Properties).</p>	<p>1. Open the workflow in <b>KNIME</b>.</p> <p>The example workflow has the following properties:</p> <ul style="list-style-type: none"><li>• Input: 2D compound structures</li><li>• Output: string, number columns and/or one 3D compound structure column.</li></ul> <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>The diagram shows: <b>SDF Reader</b> (Compound structures from the LiveReport) → <b>Credentials Configuration</b> (LiveDesign) → <b>Upload as LiveDesign Model</b>.</p>	<ol style="list-style-type: none"><li>2. Use the <b>SDF reader</b> node as input</li><li>3. Label it with "<b>LiveReport</b>". It will read the structures from the LiveReport when the workflow is run in LiveDesign.</li><li>4. Replace the output node(s) with the <b>Upload model to LiveDesign node</b></li><li>5. Add a <b>Credential Configuration</b> node.</li></ol>
 <p>The diagram shows a more complex workflow: <b>SDF Reader</b> (Compound structures from the LiveReport) → <b>LigPrep</b> (Generate 3D coordinates) → <b>QikProp</b> → <b>Column Filter</b> (Only relevant columns for the LiveReport) → <b>Save Workflow</b> (Before uploading) → <b>Credentials Configuration</b> (LiveDesign) → <b>Upload as LiveDesign Model</b> (New LiveReport column(s) - a selection of Qikprop properties).</p>	<ol style="list-style-type: none"><li>6. Save your workflow before configuring and executing the <b>Upload</b> node. It will create or update the corresponding LiveDesign model. The computational model is named after the KNIME workflow.</li></ol>



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.