

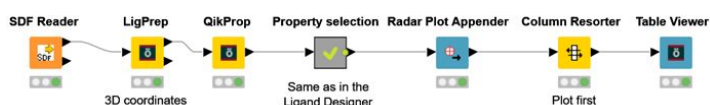
Turn a KNIME workflow into a computational model

Created with: Release 8.9

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

With KNIME, you can automate actions that you would normally do manually in Maestro. You can deploy KNIME workflows as computational models in LiveDesign. This tutorial shows how you can create a KNIME workflow that reads structures from LiveDesign, calculates properties with QikProp and uploads these properties back into LiveDesign.

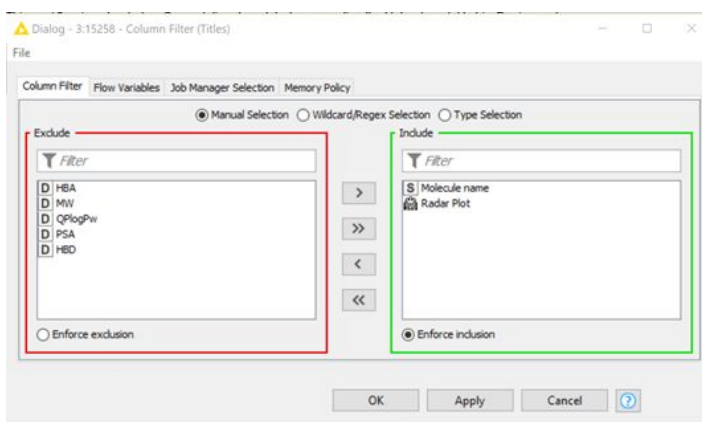
<https://kni.me/w/vpjorZ-QquJkTxPJ>



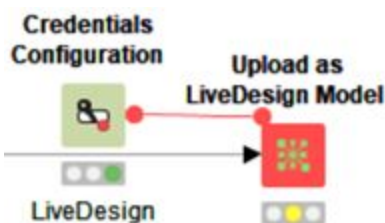
1. Download the KNIME workflow from the KNIME hub.
2. Open the **KNIME** application
3. Import the workflow by choosing **File → Import KNIME workflow**



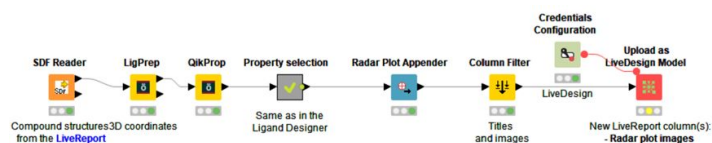
4. Check, that the reader node is an **SDF Reader** node
5. Add the label "**LiveReport**" to the node's comment. This will enable the workflow to read structures from the Live Report when you run this workflow in LiveDesign



6. Add a **Column filter** node to the workflow
7. Include only the columns containing the corporate ID, and the columns you want to add to the Live Report.

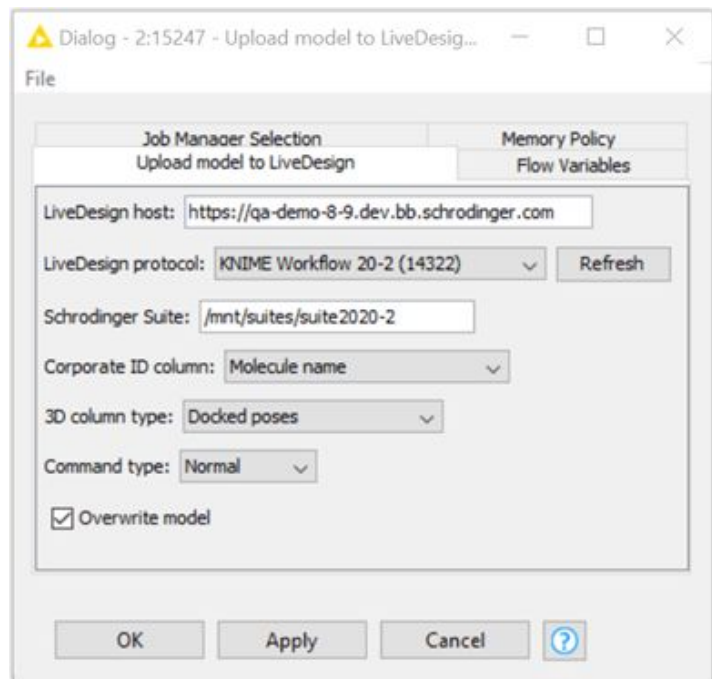


8. In the workflow, replace the **Table Viewer** node with the **Upload as LiveDesign Model** node
9. Add a **Credential Configuration** node and store your LiveDesign credentials in a variable **Id_credentials**



10. Save the workflow

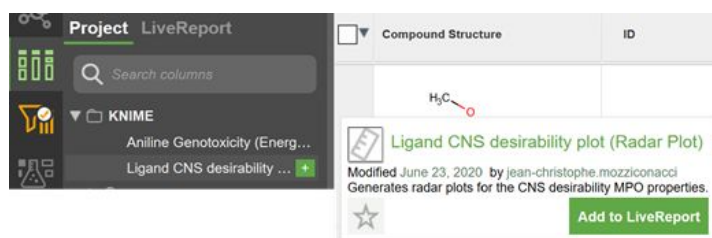
Note: The computational model is named after the KNIME workflow



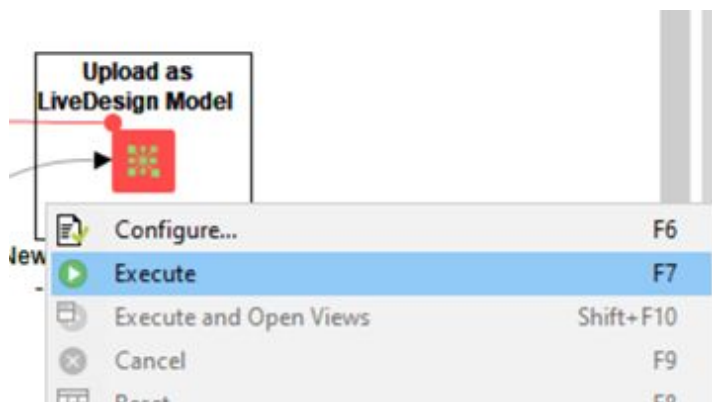
11. Configure the **Upload as LiveDesign Model** node:

- Enter the hostname of your LiveDesign instance
- Select LiveDesign protocol
KNIME Workflow 20-3
- Select the column containing the corporate ID

12. Run the **Upload as LiveDesign Model** node. The address of the computational model created or updated is printed in the KNIME console.



13. Find the computational model in the **KNIME** folder in the **Computational model** section of your LiveDesign instance.



14. In **KNIME**, edit the workflow to change the QikProp properties displayed on the radar plot.

15. Update the computational model by executing the **Upload as LiveDesign Model** node again.