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 SDF Reader LigPrep QikProp Property selection Reader Column Resorter Table Viewer SDF Reader LigPrep QikProp Property selection Radar Plot Appender Column Resorter Table Viewer Soft Same as in the Same as in the Same as in the Plot first | Download the KNIME workflow from the KNIME hub. Open the KNIME application Import the workflow by choosing File → Import KNIME workflow |
|---|---|
| SDF Reader | Check, that the reader node is an SDF Reader node 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 |
| Dialog - 3:15258 - Column Filter (Titles) File Column Filter Flow Variables Job Manager Selection Memory Policy | Add a Column filter node to the workflow Include only the columns containing the corporate ID, and the columns you want to add to the Live Report. |
| Credentials Configuration Upload as LiveDesign Model | In the workflow, replace the Table Viewer node with the Upload as LiveDesign Model node Add a Credential Configuration node and store your LiveDesign credentials in a variable Id_credentials |

| Credentials Configuration | 10. Save the workflow |
|---|---|
| SDF Reader LigPrep QikProp Property selection Radar Piot Appender Column Filter Column Filter Column filter Column filter Compound as as in the Ligand Designer Titles New LiveReport column(s): from the LiveReport | <i>Note:</i> The computational model is named after the KNIME workflow |
| Dialog - 2:15247 - Upload model to LiveDesig File Job Manager Selection Memory Policy Upload model to LiveDesign 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/suite 2020-2 Corporate ID column: Molecule name 3D column type: Docked poses Command type: Normal OK Apply Cancel ? | 11. Configure the Upload as LiveDesign Model node: a. Enter the hostname of your LiveDesign instance b. Select LiveDesign protocol KNIME Workflow 20-3 c. 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. |
| Project LiveReport ID ID ID ID ID ID | 13. Find the computational model in the KNIME folder in the Computational model section of your LiveDesign instance. |
| Upload as LiveDesign Model | 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 |
| LEV Configure F6 | |
| Execute F7 | |
| Execute and Open Views Shift+F10 | |
| Cancel F9 | |
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