

Open for Innovation

**KNIME**

# **Welcome to Interactive Web Applications**

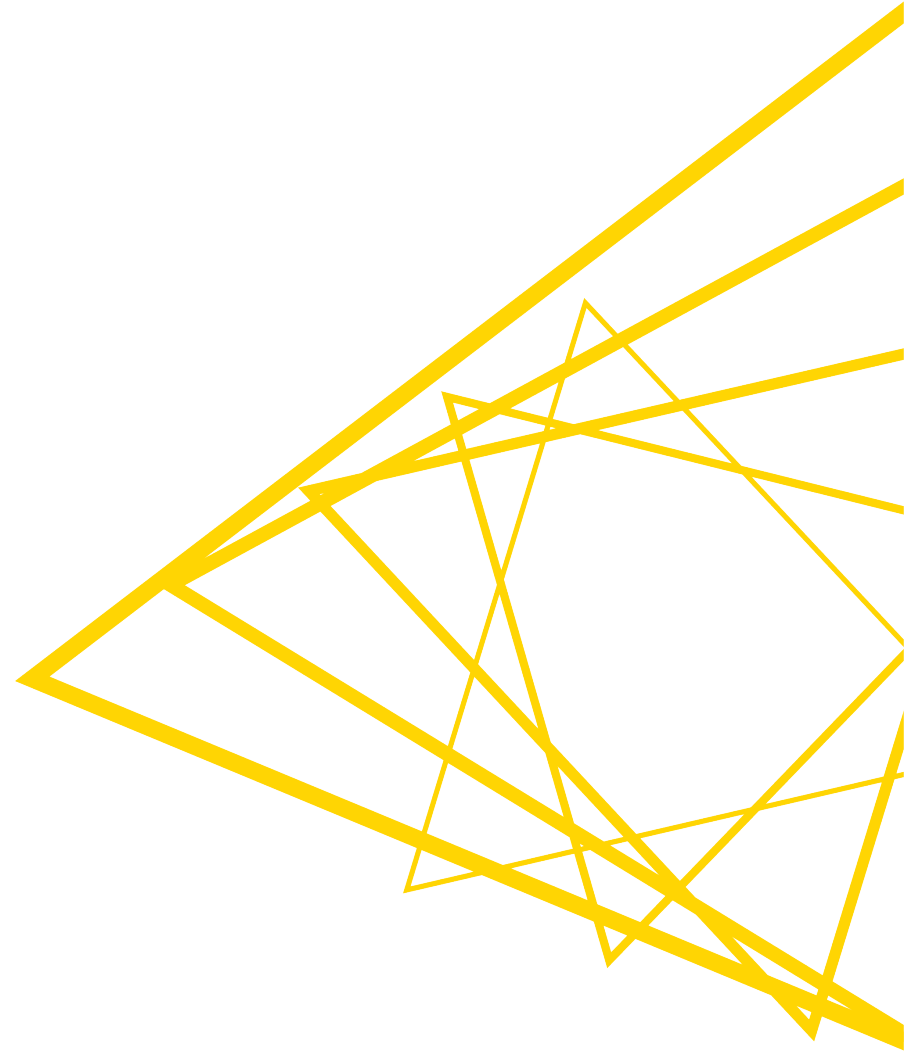
**Going live at:**

**Chicago 10:00 am**

**San Francisco 8:00 am**

**New York 11:00 am**

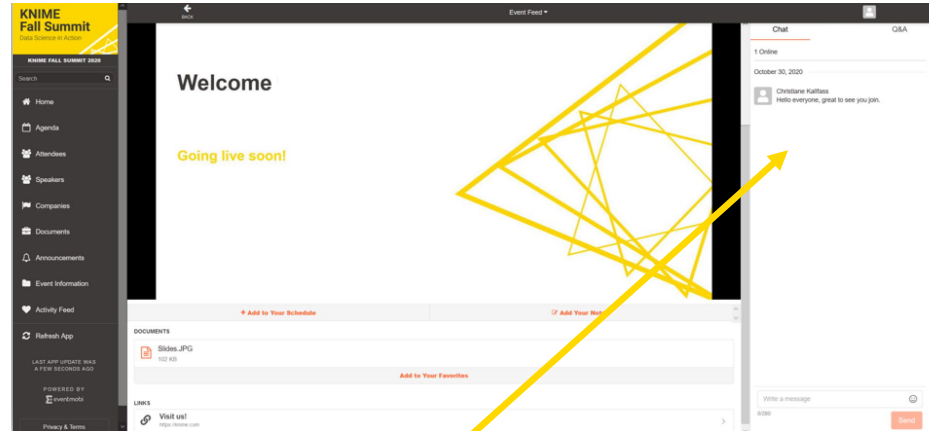
**Berlin 5:00 pm**



# Housekeeping

- Post in the chat where you are dialing in from and discuss with other attendees
- Questions? Post them in the Q&A

Questions will be answered after the presentation.



# Goal of this Workshop

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- Build an engaging web application
- Learn how to create an interactive view
  - JavaScript Views
  - Widgets
- Deploy your web application workflow to KNIME Server
- Tipps & Tricks
  - File Upload
  - Shared Components
  - Error Handling
  - Layout Editor
  - Enable Highlighting
  - Theming

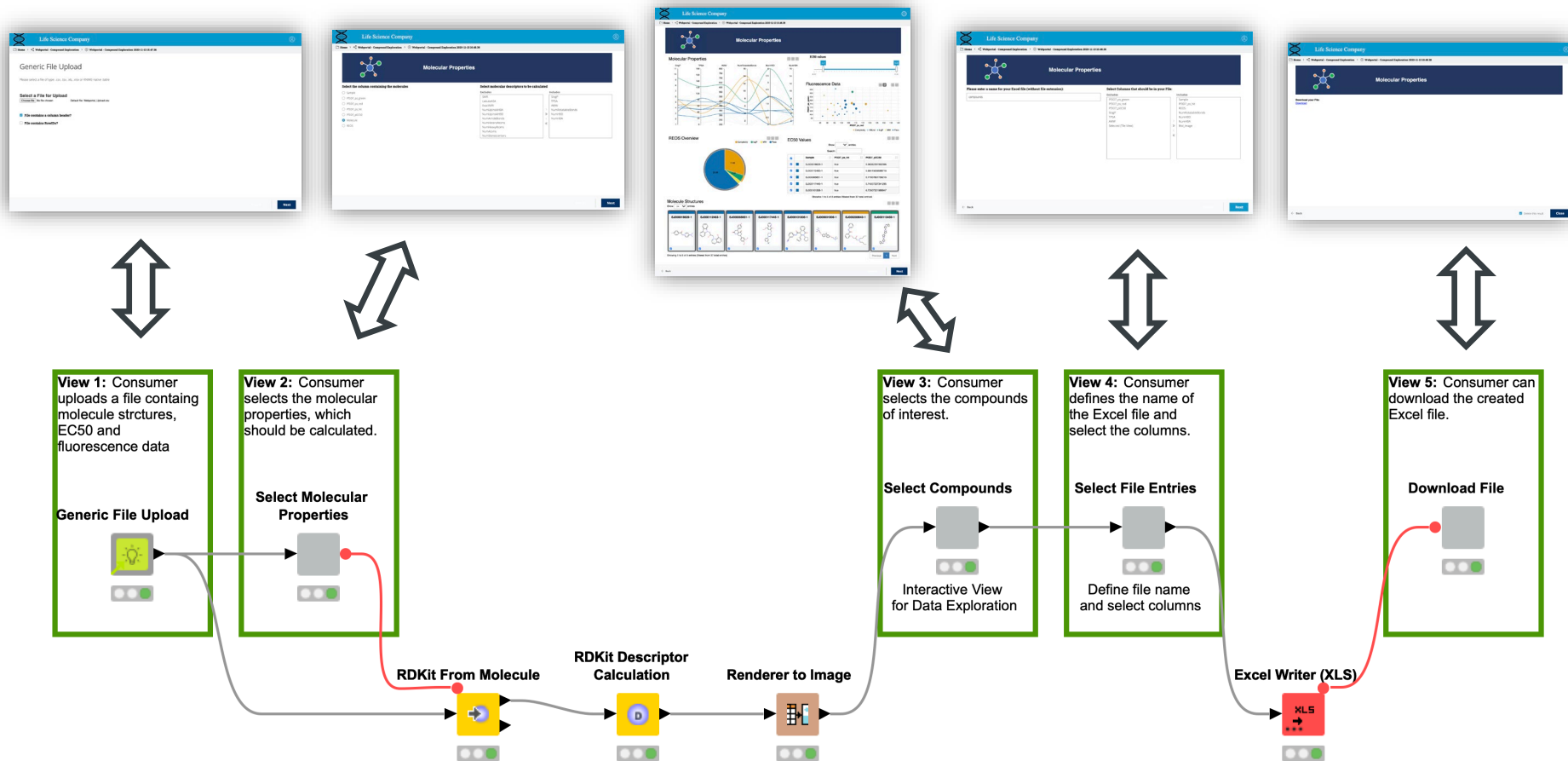
# Goal of this Workshop

## Short Demo

The screenshots show the following steps in the application:

- Generic File Upload:** A screen where users can select a file for upload. It includes options for file type and whether the file contains a column header or RowIDs.
- Molecular Properties Selection:** A screen where users select the column containing the molecules. The 'Molecule' option is selected.
- Main Dashboard:** A comprehensive view showing:
  - Molecular Properties:** A line chart with multiple data series (TPSA, AMW, NumHofmannLipinski, NumROD, NumRA) plotted against a sample ID.
  - EC50 values:** A scatter plot showing EC50 values for different samples.
  - Fluorescence Data:** A scatter plot showing fluorescence intensity for different samples.
  - REOS Overview:** A pie chart showing the distribution of samples across different categories (Complexity, MW, PPIres).
  - EC50 Values Table:** A table listing sample IDs, PPSD pH, and PPSD EC50 values.
  - Molecule Structures:** A row of chemical structures for various samples.
- Molecular Properties Export:** A screen where users can select columns to be included in an Excel export. It has 'Exclude' and 'Include' lists.

# Example Workflow



Download the Workflow here: [https://hub.knime.com/knime/spaces/Life%20Sciences/latest/Events/2020\\_11\\_20\\_KNIME\\_Summit\\_Webportal\\_Workshop/](https://hub.knime.com/knime/spaces/Life%20Sciences/latest/Events/2020_11_20_KNIME_Summit_Webportal_Workshop/)

# Interactive Views

- One component = one view
- The component needs to contain either:
  - **JavaScript nodes** for data visualization or
  - **Widget nodes** for input, selection, filter or output

The screenshot displays the KNIME Views panel, which is organized into two main sections: JavaScript and Widgets. The JavaScript section lists various data visualization views, while the Widgets section lists various interactive components.

**JavaScript Views:**

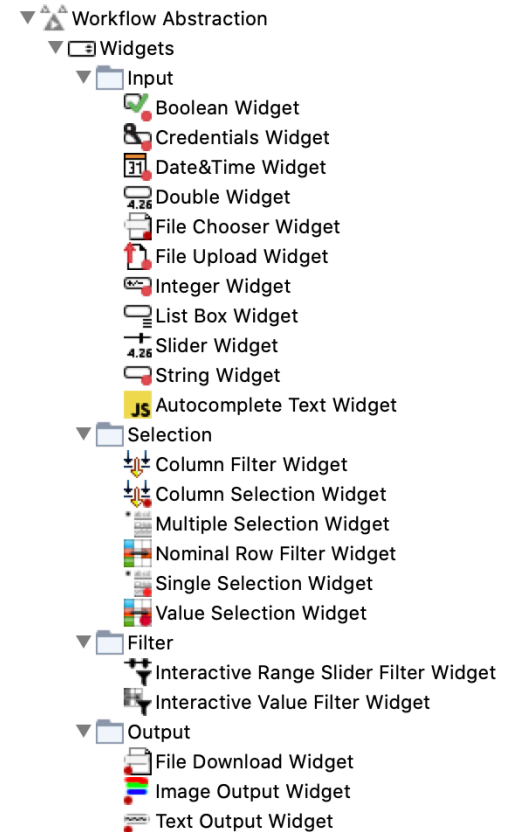
- Generic JavaScript View
- Bar Chart
- Box Plot
- Conditional Box Plot
- Decision Tree View
- Heatmap
- Histogram
- Lift Chart
- Line Plot
- Parallel Coordinates Plot
- Pie/Donut Chart
- ROC Curve
- Scatter Plot
- Stacked Area Chart
- Sunburst Chart
- Table Editor
- Table View
- Tag Cloud
- Tile View

**Widget Categories:**

- Workflow Abstraction
  - Workflow Invocation
  - Configuration
- Widgets
  - Input
    - Boolean Widget
    - Credentials Widget
    - Date&Time Widget
    - Double Widget
    - File Chooser Widget
    - File Upload Widget
    - Integer Widget
    - List Box Widget
    - Slider Widget
    - String Widget
    - Autocomplete Text Widget
  - Selection
    - Column Filter Widget
    - Column Selection Widget
    - Multiple Selection Widget
    - Nominal Row Filter Widget
    - Single Selection Widget
    - Value Selection Widget
  - Filter
    - Interactive Range Slider Filter Widget
    - Interactive Value Filter Widget
  - Output
    - File Download Widget
    - Image Output Widget
    - Text Output Widget

# Widgets

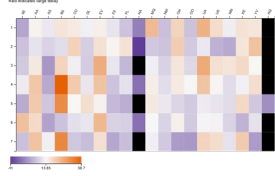
- Widget nodes for
  - Input
  - Selection
  - Filter
  - Output
- Widget nodes are corresponding to the Configuration nodes for the WebPortal
- Provide basic validation of input



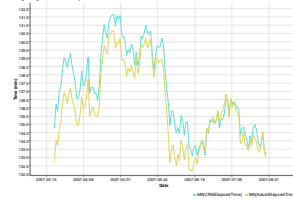
# JavaScript nodes: Data Visualization

- Large selection of easy-to-use visualization nodes
  - Web-based and interactive
  - Dedicated nodes, no scripting required

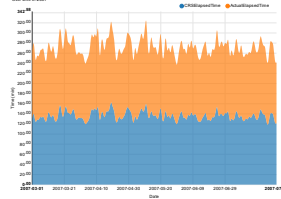
Delay Times by Day of the Week and Carrier



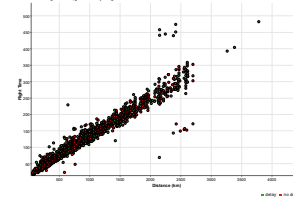
Actual Elapsed Time vs CRS Elapsed Time



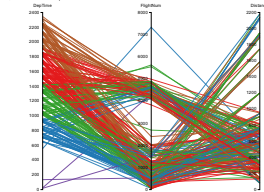
Actual Elapsed Time and CRS Elapsed Time



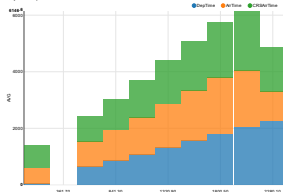
Correlation between Distance and Flight Time



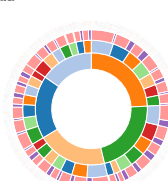
Departure Time vs Flight Number vs Distance



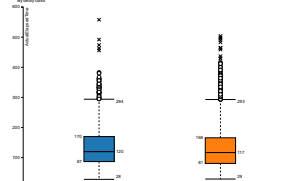
Average Arrival Time and CRS Arrival Time



Flights by Delay Status, Month, and Day of the Week



Distribution of Elapsed Time



Views

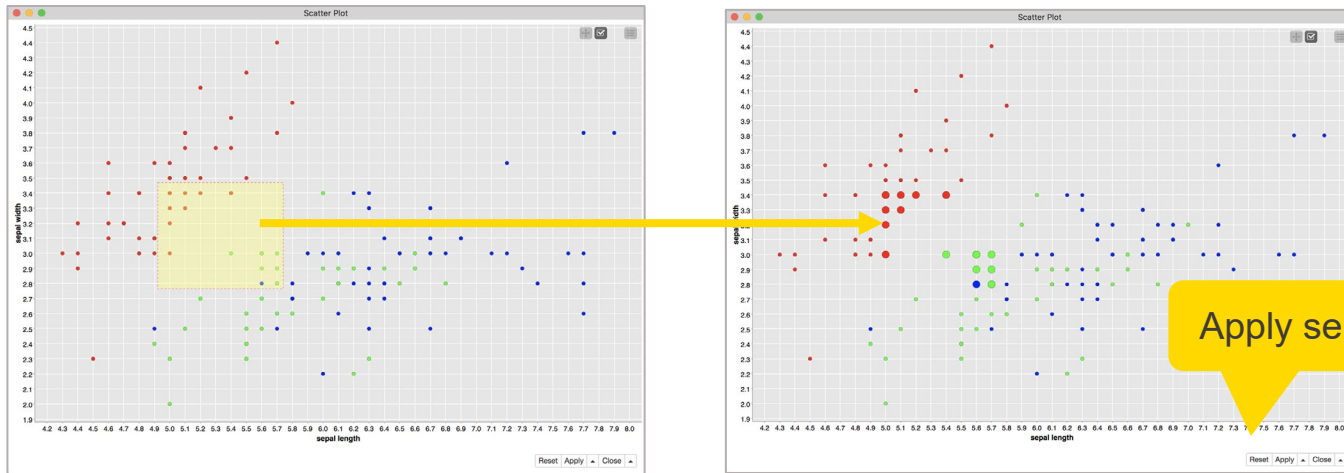
- JavaScript
  - Generic JavaScript View
  - Bar Chart
  - Box Plot
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  - Decision Tree View
  - Heatmap
  - Histogram
  - Lift Chart
  - Line Plot
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  - Stacked Area Chart
  - Sunburst Chart
  - Table Editor
  - Table View
  - Tag Cloud
  - Tile View



# Selection & Filtering in JavaScript Views

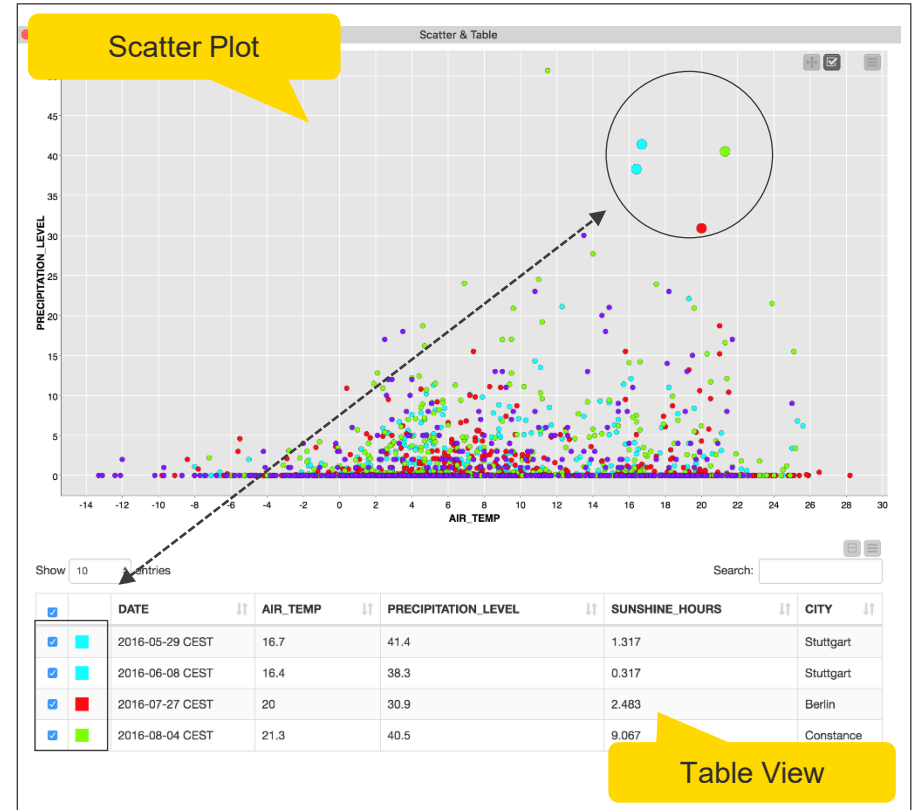
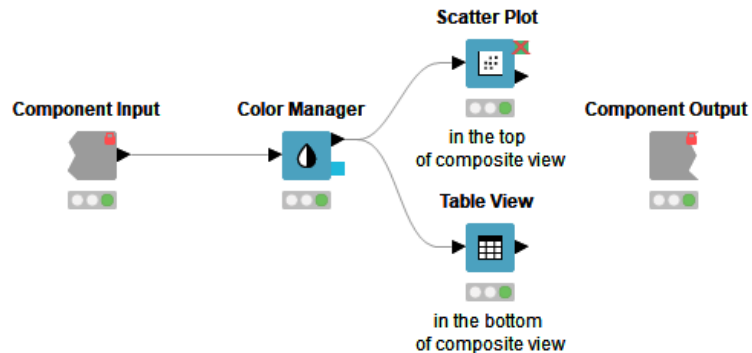
Interactivity allows you to select data points in views

- Selection is propagated to other views.
- Highlight selected rows or filter them
- Click “Apply” to add column to data that indicates selection (true/false) for use in downstream nodes

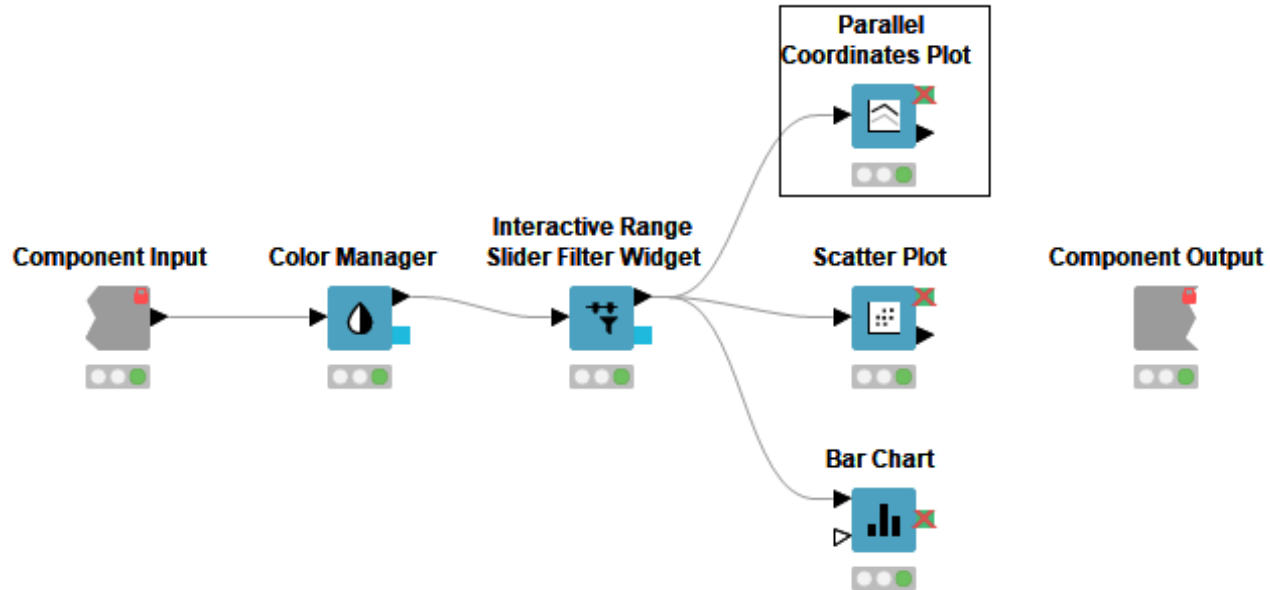


# Components – Combined Views

- Multiple JavaScript View nodes can be combined in Components
- Selections are transmitted to all other views
- Also for use on the KNIME WebPortal



# Interactivity across Charts: Selection and Filter Events



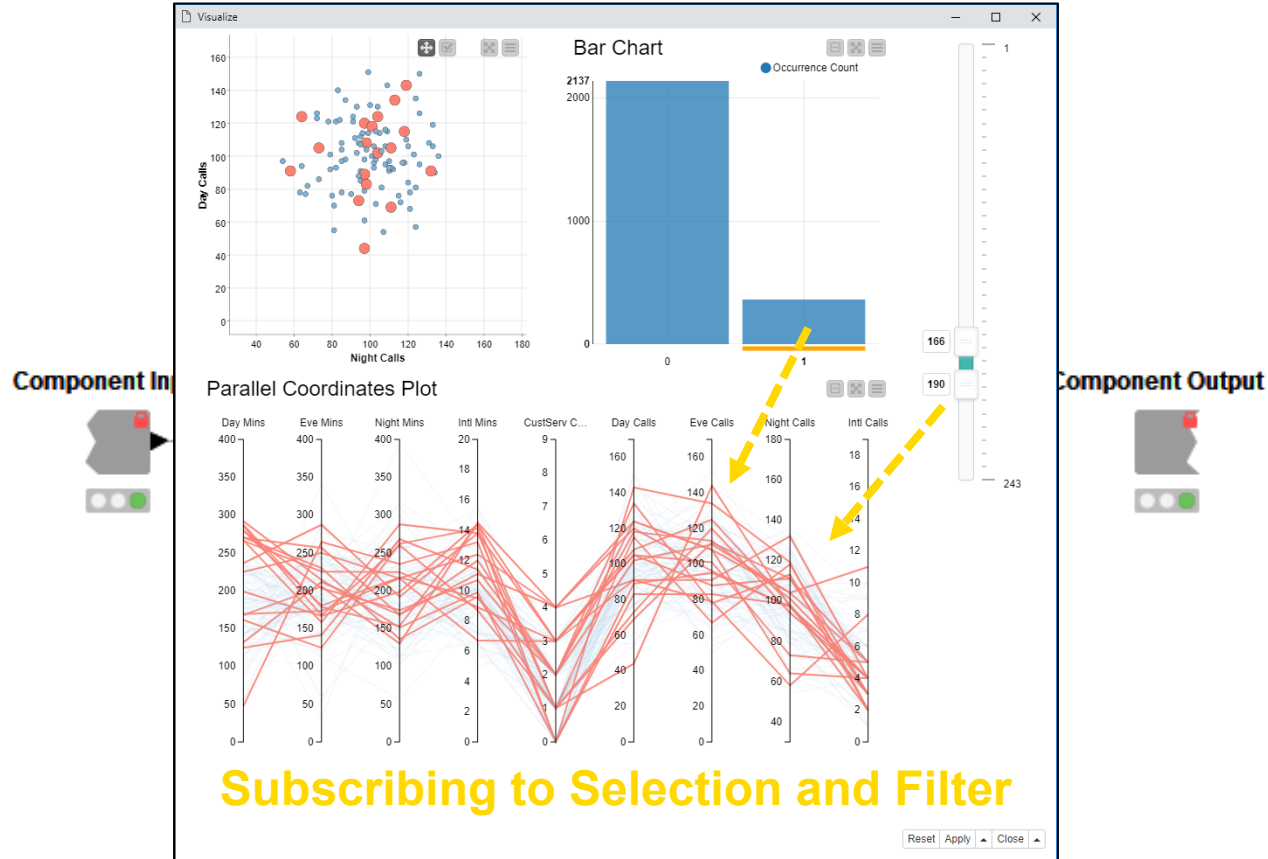
# Interactivity across Charts: Selection and Filter Events

The image shows a dialog box titled "Dialog - 6:17:0:15 - Parallel Coordinates Plot ...". The dialog has a "File" menu and several tabs: "Options", "General Plot Options", and "Control Options". Under "Options", there are sub-tabs for "Selection and Filter", "Flow Variables", and "Memory Policy". The "Selection and Filter" sub-tab is active, showing a list of checked options:

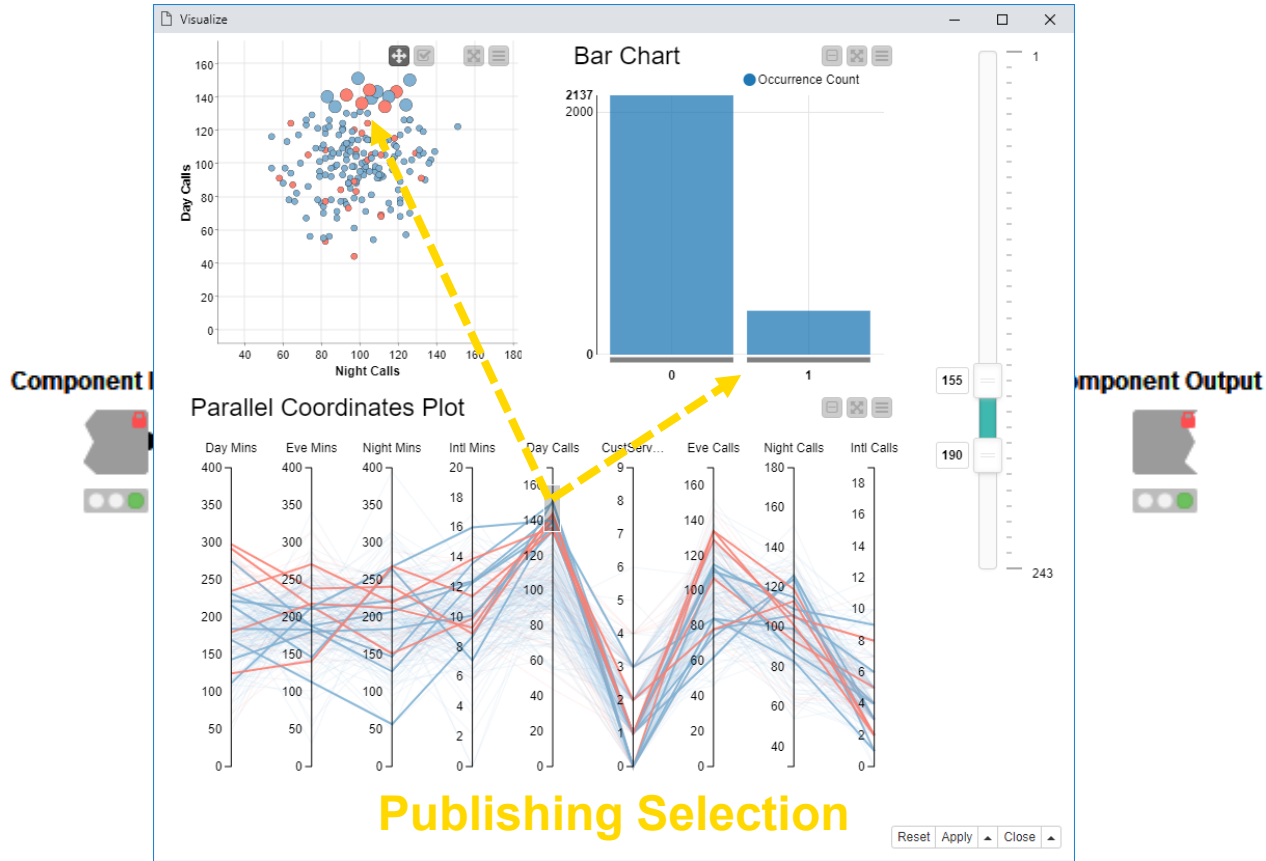
- Enable selection
- Enable range selection
- Display clear selection button
- Publish selection events
- Subscribe to selection events
- Subscribe to filter events

At the bottom of the dialog are buttons for "OK", "Apply", "Cancel", and a help icon. To the left of the dialog is a "Component Input" icon, and to the right is a "Component Output" icon, both with arrows pointing towards the dialog.

# Interactivity across Charts: Selection and Filter Events

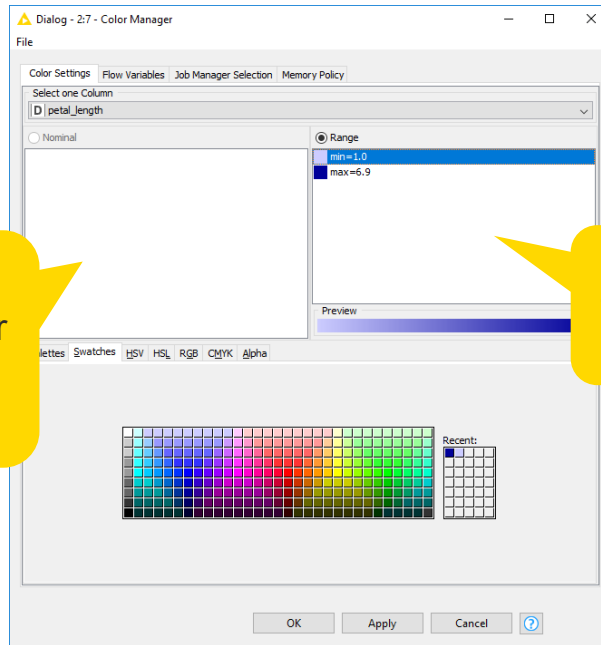


# Interactivity across Charts: Selection and Filter Events

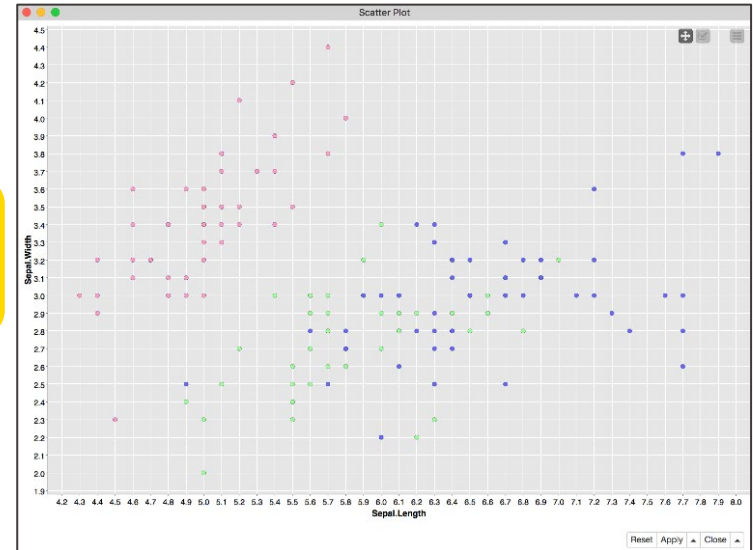
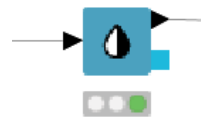


# Tipp: Color Manager

- Color by nominal or continuous values
- Sync colors between views using the color model port and Color Appender node



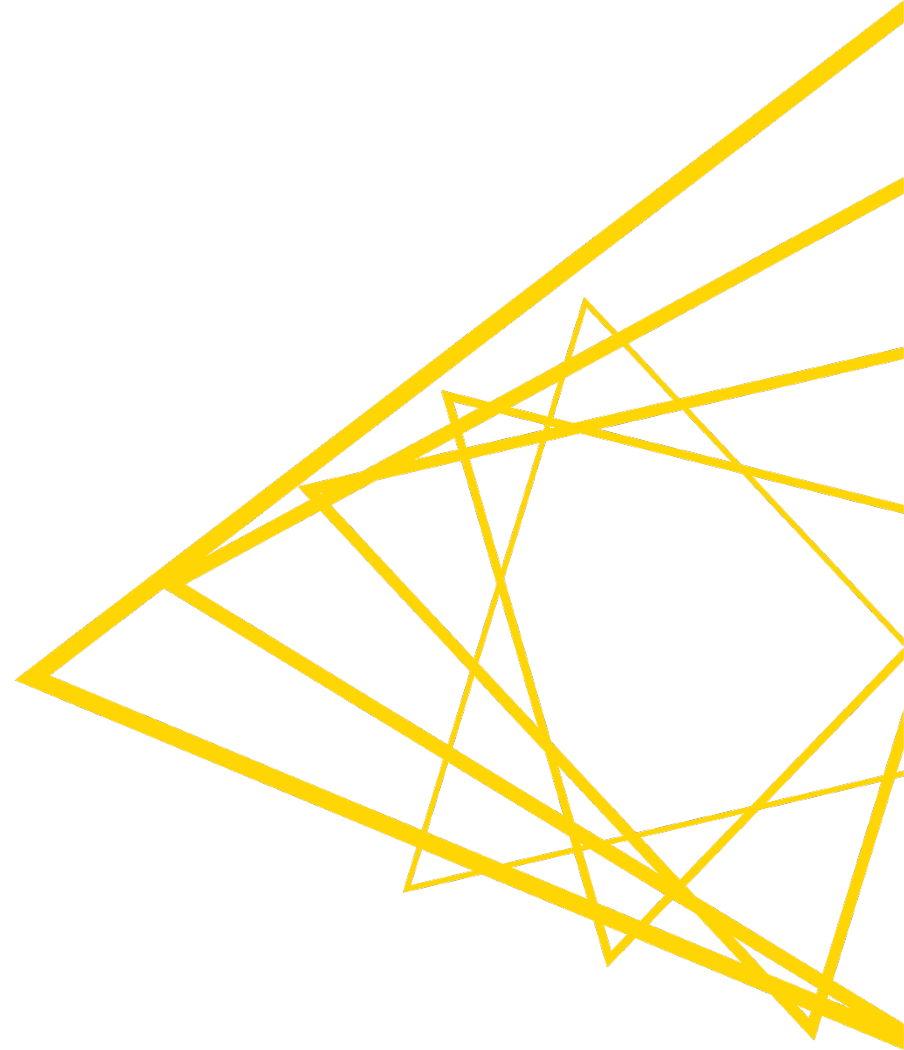
Color Manager



Discrete colors for nominal values

Color range for numerical values

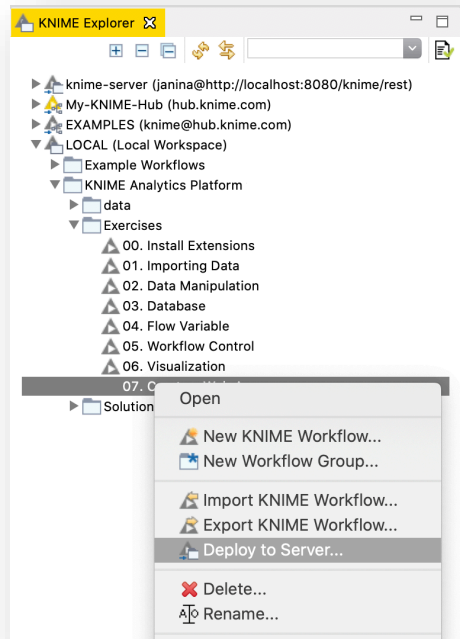
**Deploy your workflow**



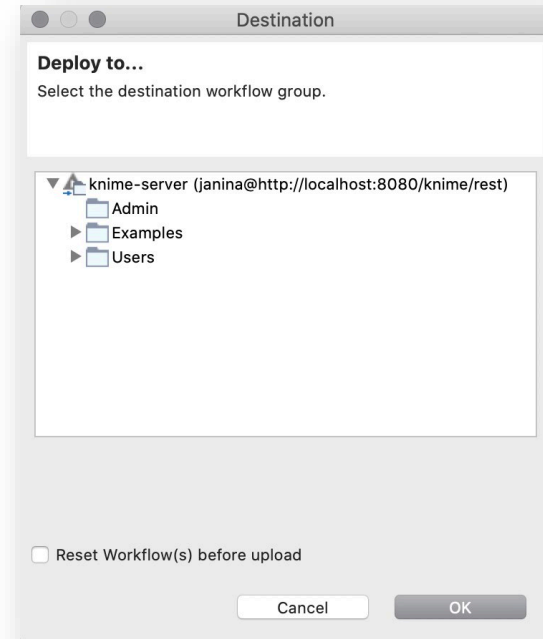


# Deploy a Workflow to the KNIME Server

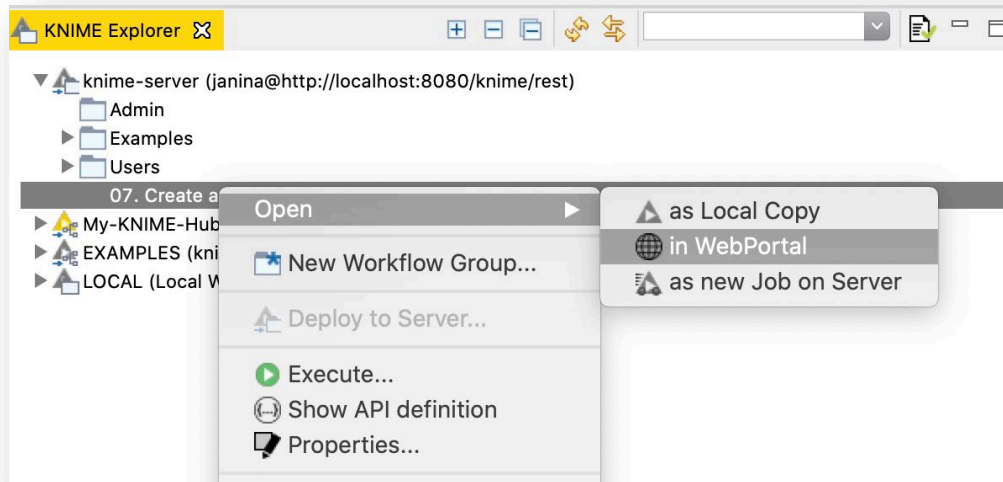
Right click on the workflow and select *Deploy to Server ...*



Select Destination on Server



# Start a Workflow from KNIME Analytics Platform



- *As Local Copy*: Opens the workflow, which is executed locally
- *In WebPortal*: Opens the KNIME WebPortal in a Browser, where the workflow is executed on the KNIME Server and the views for the Web app are shown in the Browser
- *As new Job on Server*: Creates a job, which is executed on the Server.

# Start a Workflow directly in a Browser

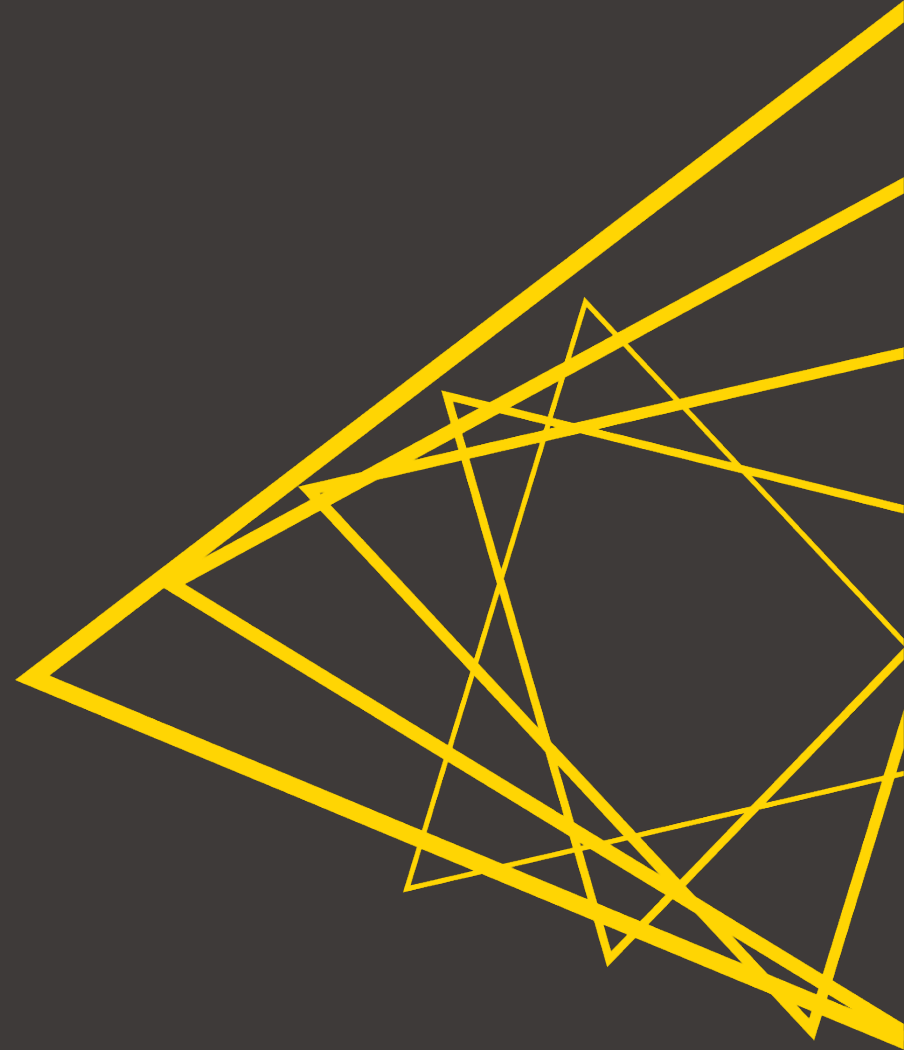
A workflow can also be started with a direct link (new WebPortal):

`http://<server-address>/knime/webportal/space/<ItemPath>?exec<WorkflowParameters>`

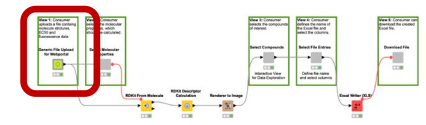
The screenshot shows the Knime WebPortal interface. At the top, there is a blue header with a DNA double helix icon, the text 'Life Science Company', and a user profile icon. Below the header is a breadcrumb trail: 'Home > Webportal - Compound Exploration'. The main content area features the title 'Webportal - Compound Exploration' with a document icon. To the right of the title are three buttons: 'Copy link to...', 'Current page', and 'Run workflow'. Below the title is a paragraph of text: 'If run on the Webportal, this workflow is a simple interactive web app helping to explore potential compounds. First, the expert selects the molecular properties, which should be calculated. Second, the expert selects the compounds of interest. Third, the expert defines the name of the Excel file and which columns should be included in the Excel file. Last, the expert can download the created Excel file. TAGS: web app'. Below this text is a checkbox labeled 'Notify me when workflow has run'. At the bottom of the main content area is a dark blue button with a play icon and the text 'Run'. Below the main content area is a light gray section with a play icon and the text 'Jobs'. Underneath 'Jobs' is the text 'No jobs available'.

old Webportal: `http://<server-address>/knime/##/<ItemPath>&<WorkflowParameters>`

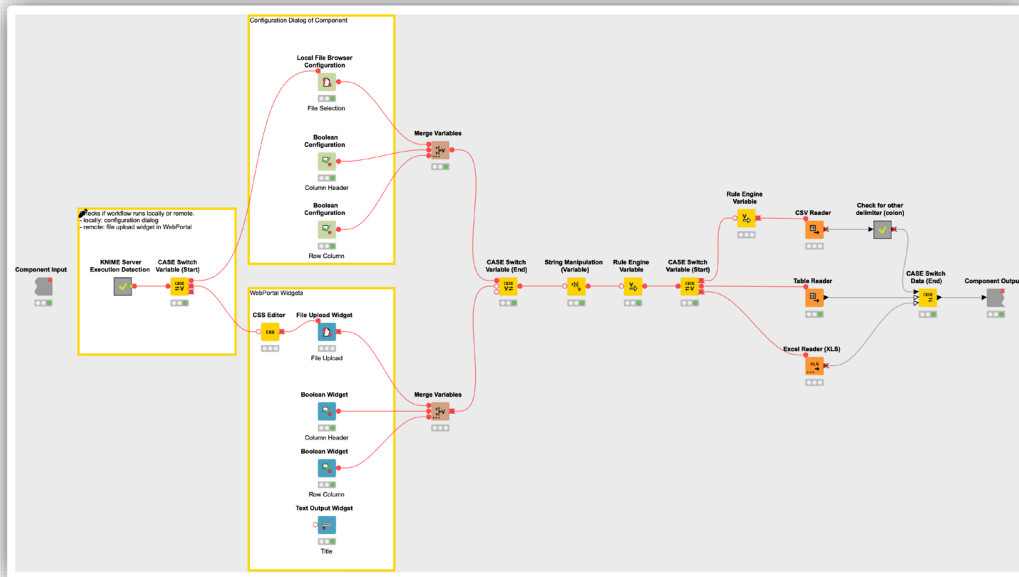
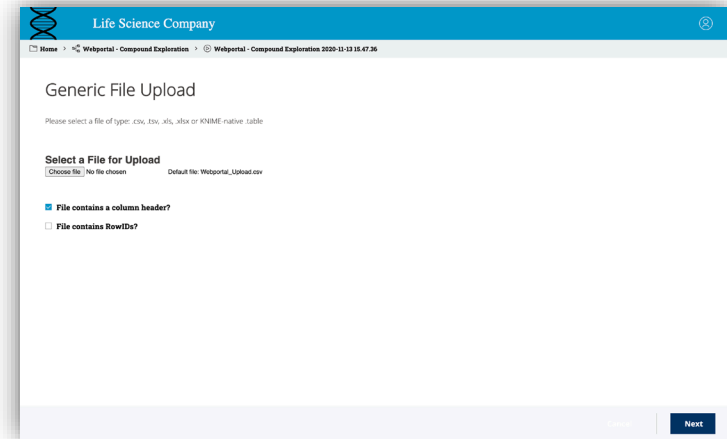
# Tipps & Tricks



# First View: Generic File Upload



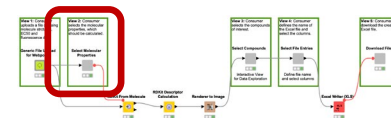
- Reused a shared component from the KNIME Hub: [Generic File Upload](#)
- Component allows to upload different file formats (csv, xlsx, table) and selects correct Reader node



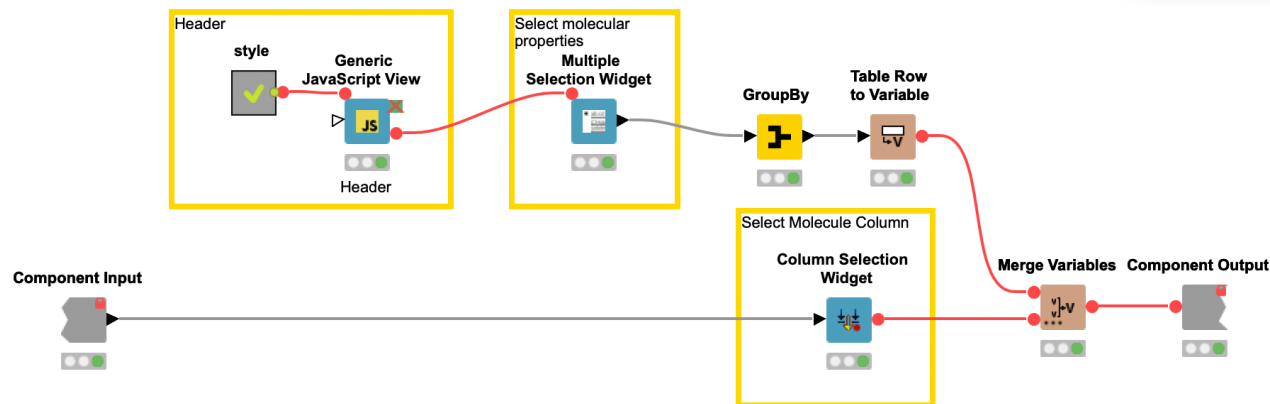
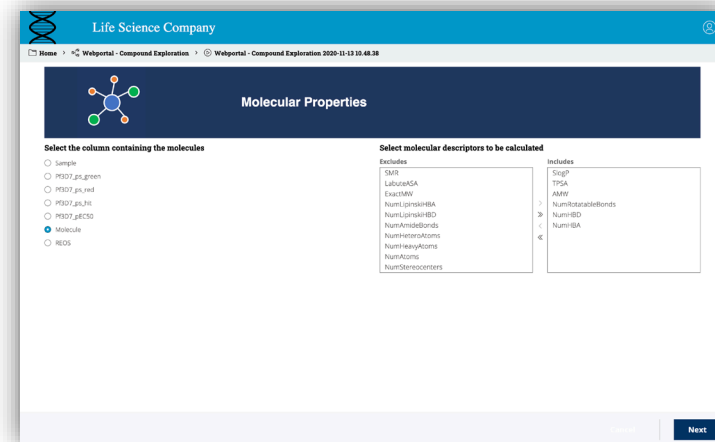
## Generic File Upload



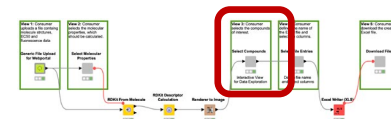
# First View: Select Molecular Properties



- Generic JavaScript View: customized header
- For user selection:
  - Multiple Selection Widget: Select which molecular properties should be calculated
  - Column Selection Widget: Select column with Molecule Structure information



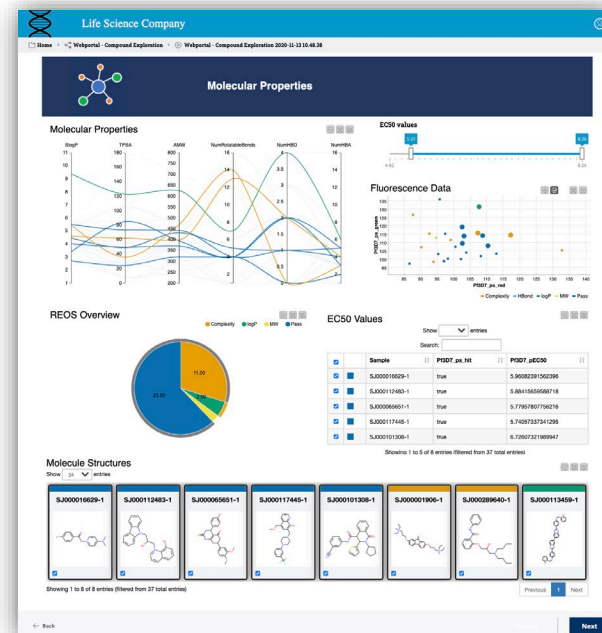
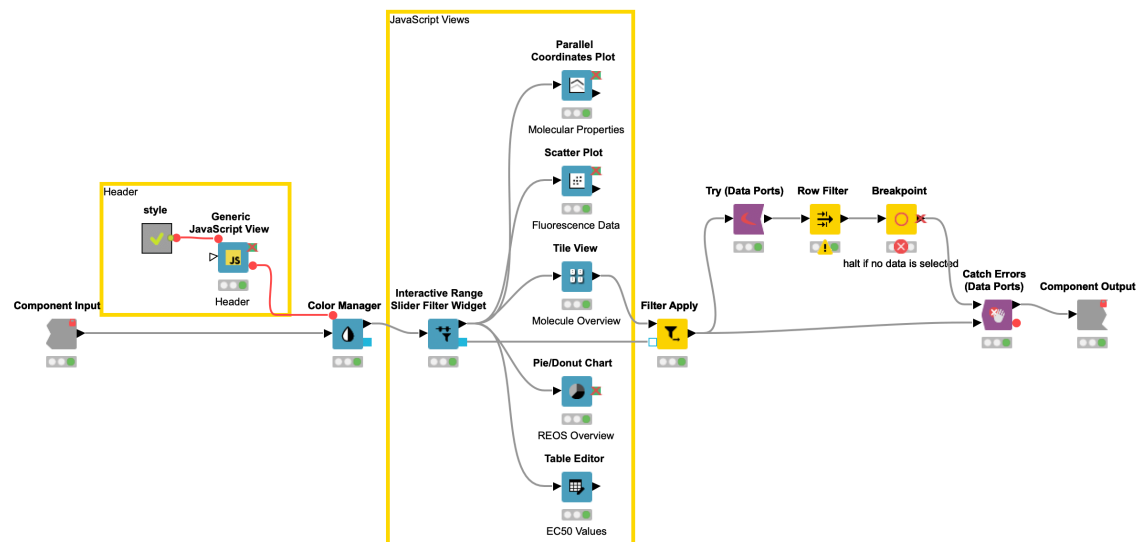
# Second View: Select Molecular Properties



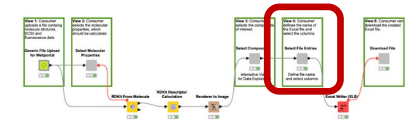
- Tipp: Use the Layout Editor to arrange the JavaScript views:



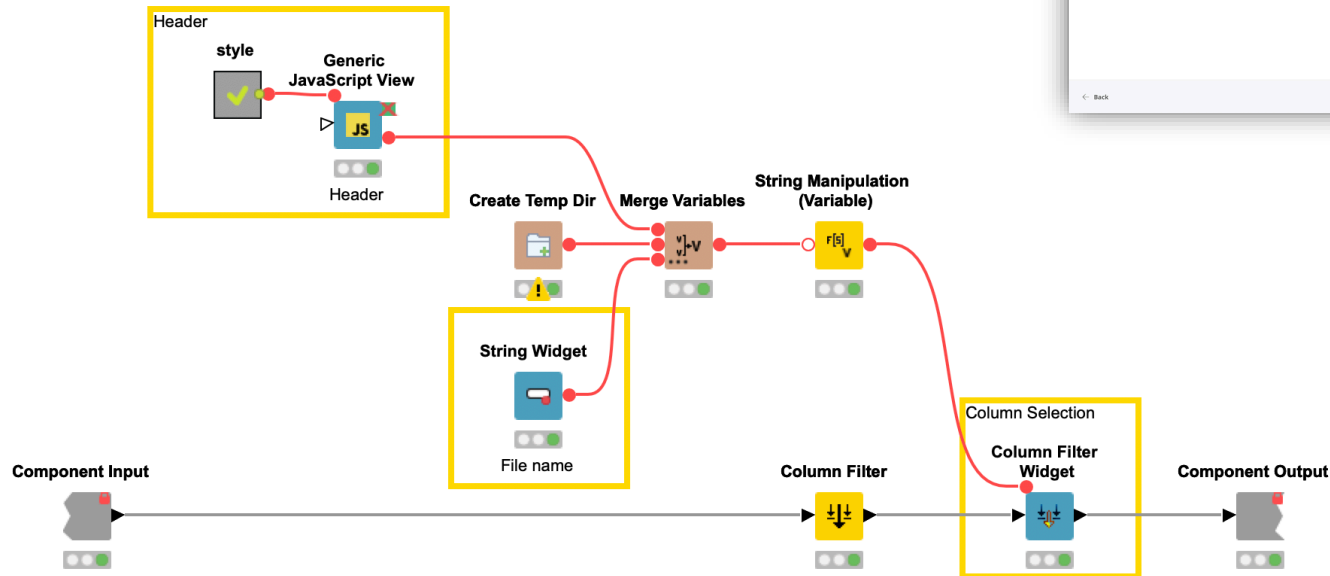
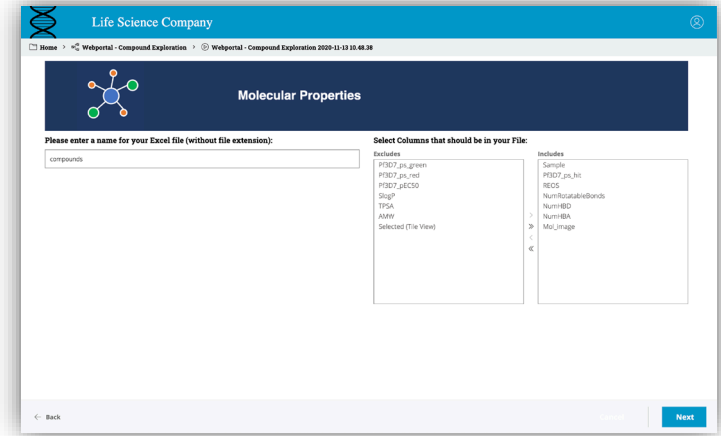
- Tipp: Use Try-Catch to account for cases where user does not select any data points



# Third View: Select File Entries

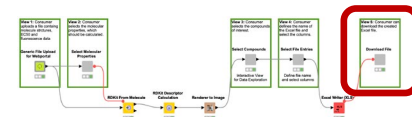


- For user input/selection:
  - String Widget: file name
  - Column Filter Widget: select columns for file

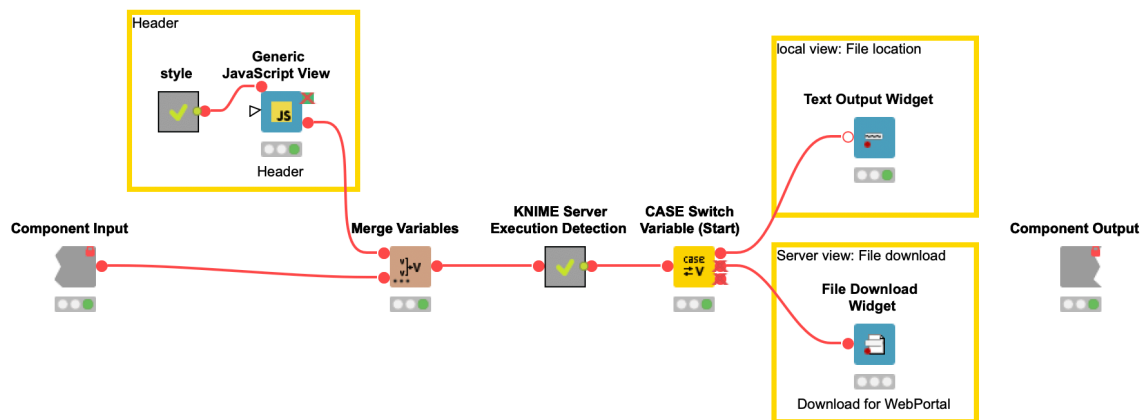




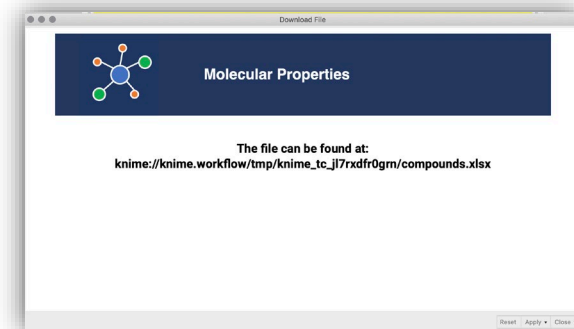
# Fourth View: File Output/Download



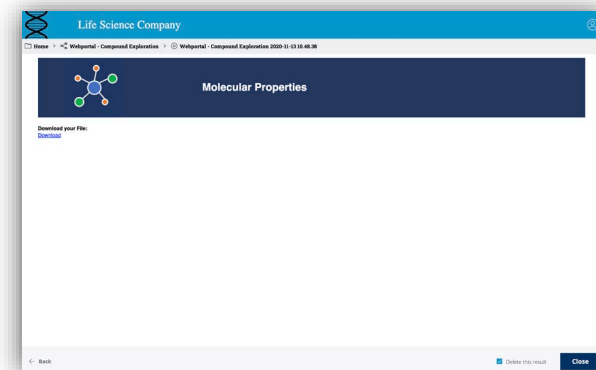
- Two different views:
  - If executed locally: File location is displayed
  - If executed remotely (WebPortal): Link to download the file



Local view:



KNIME Webportal view:



# Theming

- Apply a customized theme to the WebPortal (see [Documentation](#))

## Default Theme

KNIME WebPortal

Molecular Properties

Select the column containing the molecules

- SMILES
- PPSD\_pq\_green
- PPSD\_pq\_red
- PPSD\_pq\_blue
- PPSD\_pq\_COSY
- Molecule
- HBD

Select molecular descriptors to be calculated

Includes

- SMILES
- TPSA
- MW
- NumHeteroatoms
- NumHBD
- NumRings

## Customized Theme

Life Science Company

KNIME WebPortal

Molecular Properties

Select the column containing the molecules

- SMILES
- PPSD\_pq\_green
- PPSD\_pq\_red
- PPSD\_pq\_blue
- Molecule
- HBD

Select molecular descriptors to be calculated

Includes

- SMILES
- TPSA
- MW
- NumHeteroatoms
- NumHBD
- NumRings

KNIME WebPortal

Molecular Properties

Molecular Properties

EC50 values

Fluorescence Data

REOS Overview

EC50 Values

Cancel Next

Life Science Company

KNIME WebPortal

Molecular Properties

Molecular Properties

EC50 values

Fluorescence Data

REOS Overview

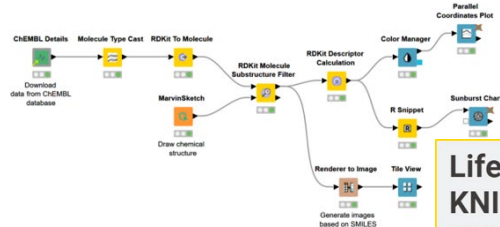
EC50 Values

Cancel Next

# Why KNIME for Life Sciences?

<https://www.knime.com/why-knime-for-life-science>

## Versatile and Open Analytics for the Life Sciences



Find out more about accessing, transforming, and interacting with large amounts of life science data.

Contact us

## Why KNIME for Life Sciences

Analytical data  
Cheminformatics Clinical data  
AI/Machine learning QA/QC Metabolomics  
Bioinformatics Genomics  
Digital pathology **Life Sciences** Text mining  
Interactive data exploration High-content screening  
Computational chemistry Multi-objective optimization  
Data integration High-throughput screening  
Competitive intelligence

Work with your specific life science data types easily and in one single environment.

Manage large amounts of data all in one place.

Take advantage of machine learning capabilities in KNIME.

Use life science community nodes such as [RDKit](#), [Vernalis](#), [SeqAn](#), and more.

Draw on expertise from the KNIME Team as well as the community via the [KNIME Forum](#).

## Life Sciences on the KNIME Blog

Scale and orchestrate the modeling process to train and evaluate 300,000 models or bioactivity prediction.

Explore, analyze, visualize: create interactive views using sunburst charts, tag clouds, and networks based on the example of investigating disease-related genes.

Learn how to use Python code found in Jupyter notebooks in KNIME as well as how to execute KNIME workflows directly from within Python.

Answer questions from the area of pharmaceutical research by linking and querying different datasets stored in BigQuery.

Visit KNIME Blog



## KNIME in Action

Examples of KNIME in Action from our community of Life Science users:

Deep Learning: From Mastering the Game of Go to Revolutionizing Microscopy - by Florian Jug (deNBI). [Open slides](#).

Building a Clinically Significant Rare Disease Data Master: Approach and Workflows - by Sebastien Lefebvre (Alexion Pharmaceuticals). [Open slides](#).

Using KNIME to Build a Data-Driven Culture (and Workflows) in a Biopharma Setting - by Kenneth Longo (WAVE Life Sciences). [Open slides](#).

# Stay connected with KNIME

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**Blog:** [knime.com/blog](https://knime.com/blog)



**Forum:** [forum.knime.com](https://forum.knime.com)



**KNIME Hub:** [hub.knime.com](https://hub.knime.com)



**KNIME E-Learning Course:**  
[www.knime.com/e-learning-course](https://www.knime.com/e-learning-course)

Follow us on social media:



# KNIME Books

Course books are available on **KNIME Press**

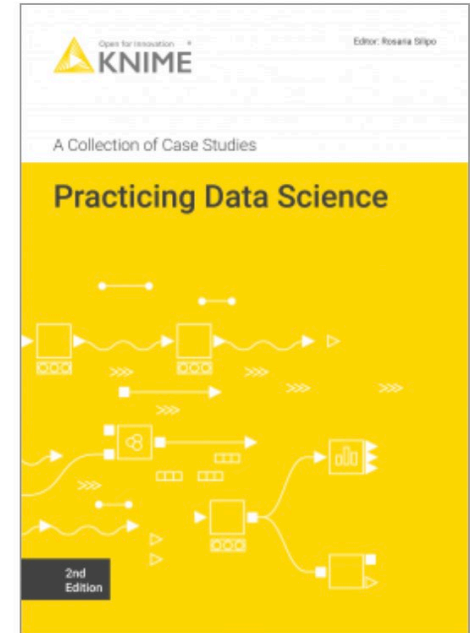
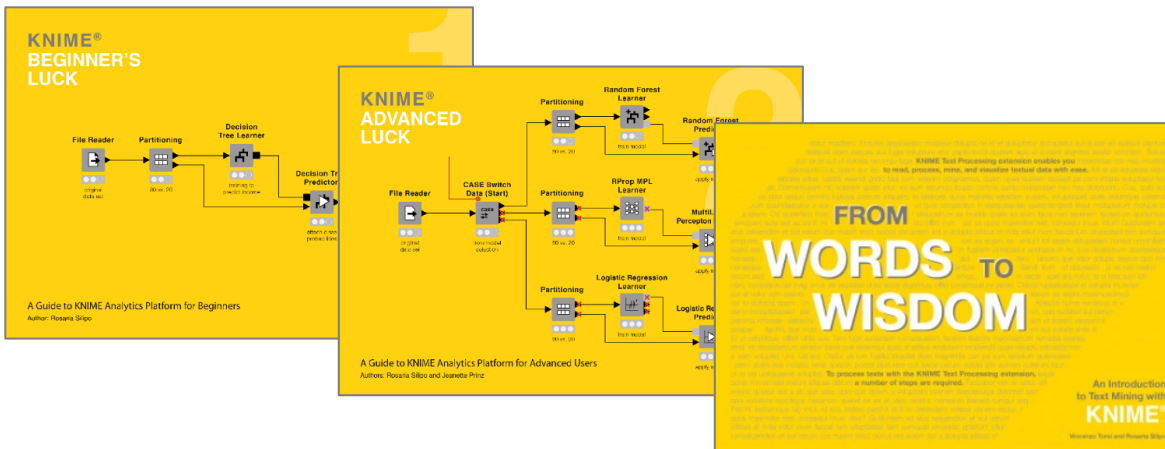
<https://www.knime.com/knimepress>

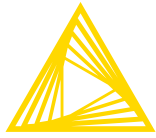
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Open for Innovation

**KNIME**

**Thank you for joining!**

