

# KNIME: The COSMOS Integration Platform



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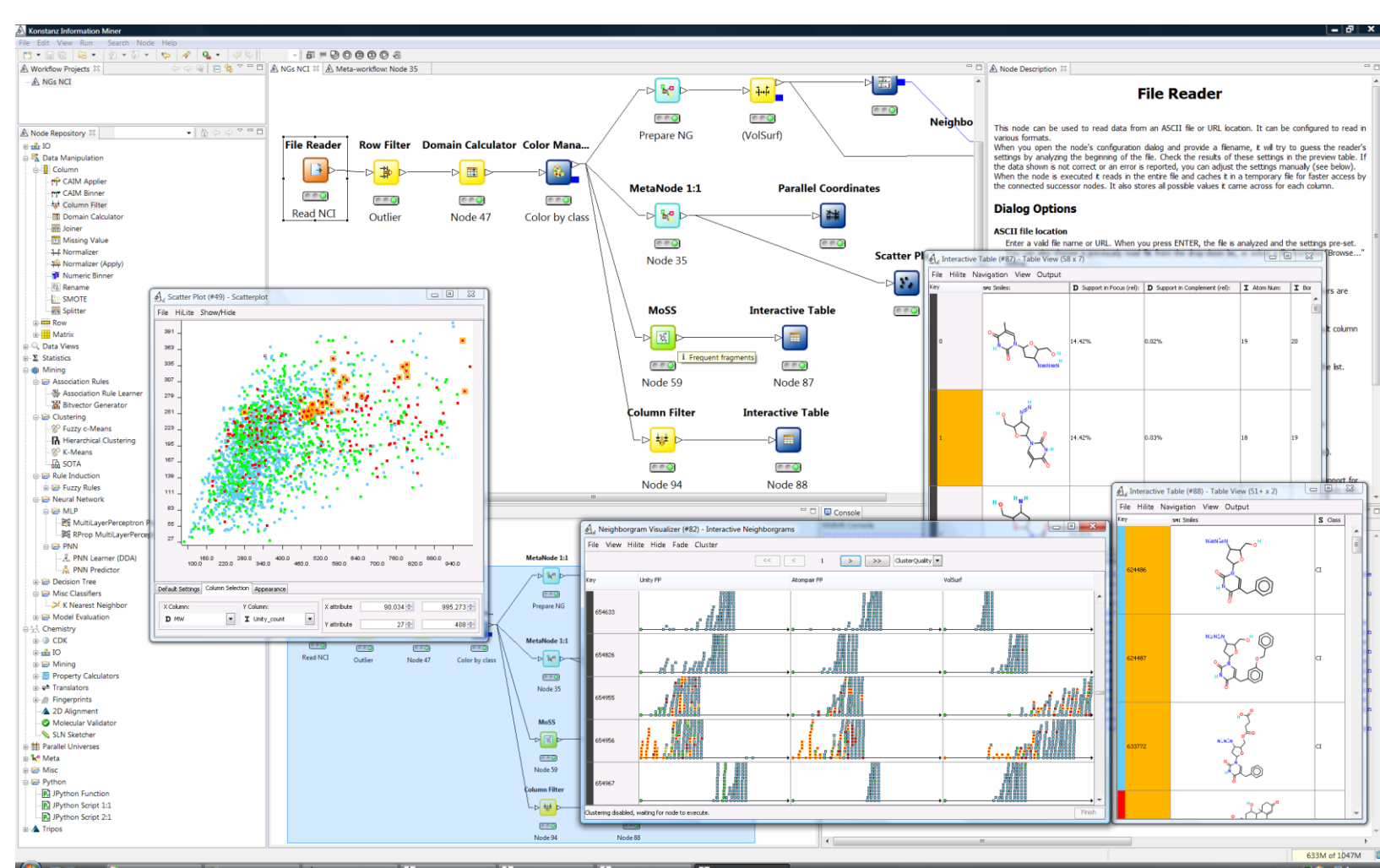
## Introduction and Aims

KNIME is used as the integration platform for the predictive toxicology methods and database which are being developed in the COSMOS project. By means of graphical workflows, data are read from various data sources and subsequently transformed into suitable formats for model building and/or visual analysis.

KNIME workflows will be freely available and provide a transparent method to assess the toxicity of cosmetics.

## What is KNIME?

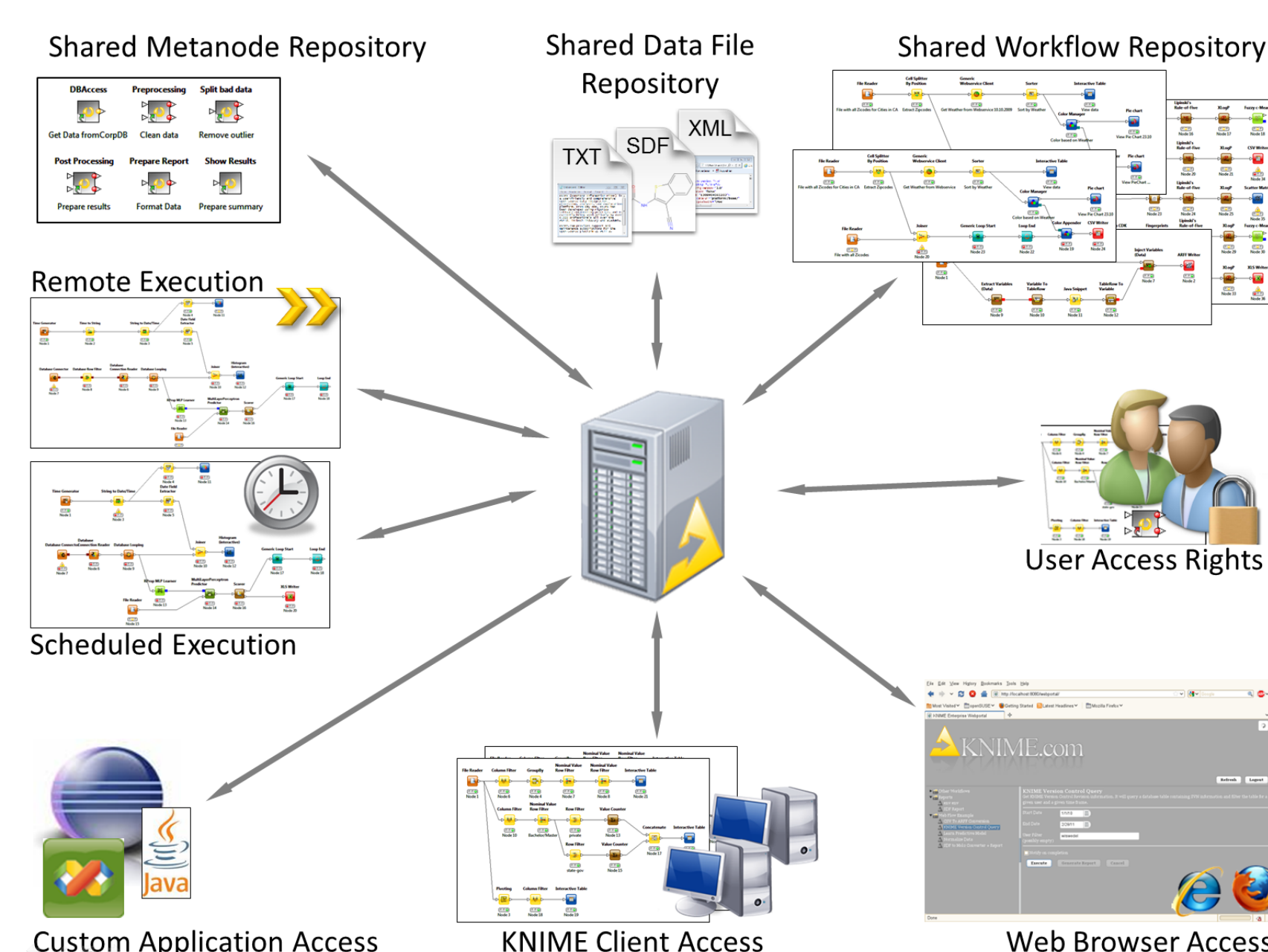
- Open-source data mining platform with intuitive graphical user interface (GUI)
- Building graphical predictive workflows with hundreds of standard operators (nodes)
- Data is read from various data sources, such as databases, text files, chemical structure files, excel files, XML, web services, etc.
- Data is passed along processing nodes in a table format and is stored with workflow for documentation
- Intermediate and final results can be inspected at any time with various kinds of interactive visualisations
- Easily extensible through a well-defined and slim application programming interface (API)
- Additional functionality easily installable from KNIME, from a large open-source community or from commercial software vendors: image processing, time series analysis, network analysis, text processing and information retrieval, chemoinformatics, bioinformatics
- Reporting tool creates result sheets from the data as PDF, DOC, PPT, etc. through open-source BIRT engine



## Requirements for COSMOS

- Easy integration of new methods, models and flows - usually by means of new implementation of nodes
- Sharing of methods and complete workflows via a central repository
- Collaborative development of new workflows
- Providing workflows to end-users via a simple (web-based) frontend
- Versioning and archival of workflows
- Open technology that does not restrict usage by end-users

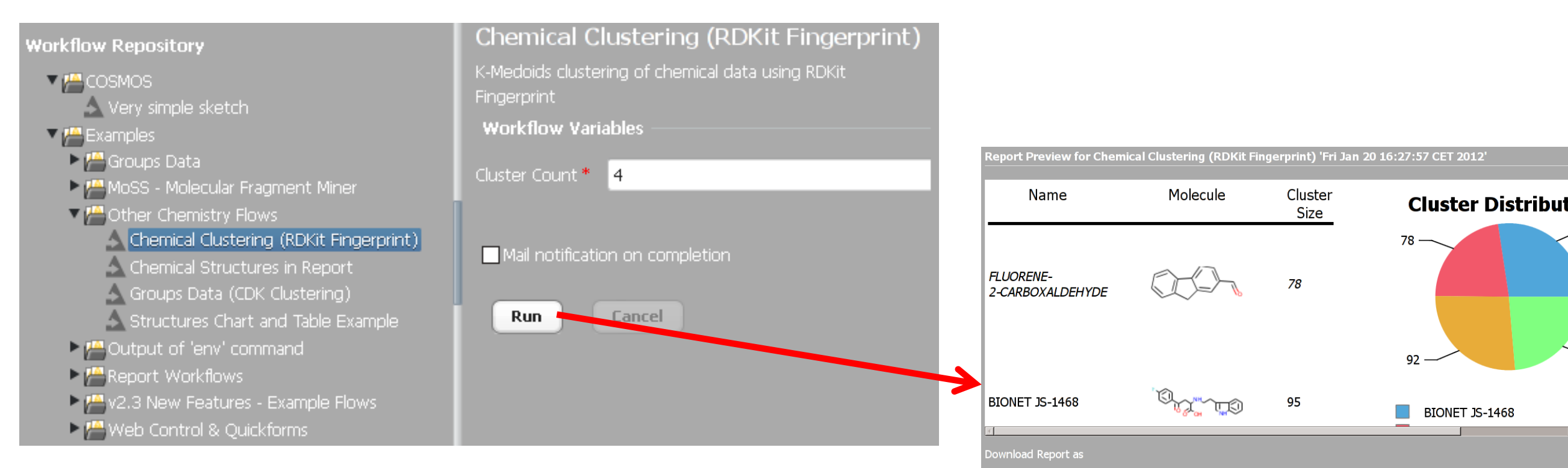
## KNIME Enterprise Server



- Central repository to share KNIME workflows
  - Up- and download workflows
  - Execute workflows on the server
  - User access control. Permissions per login user.
  - Hosts Metanode Templates: re-usable sub-workflows
- Integrated in the intuitive KNIME Client GUI

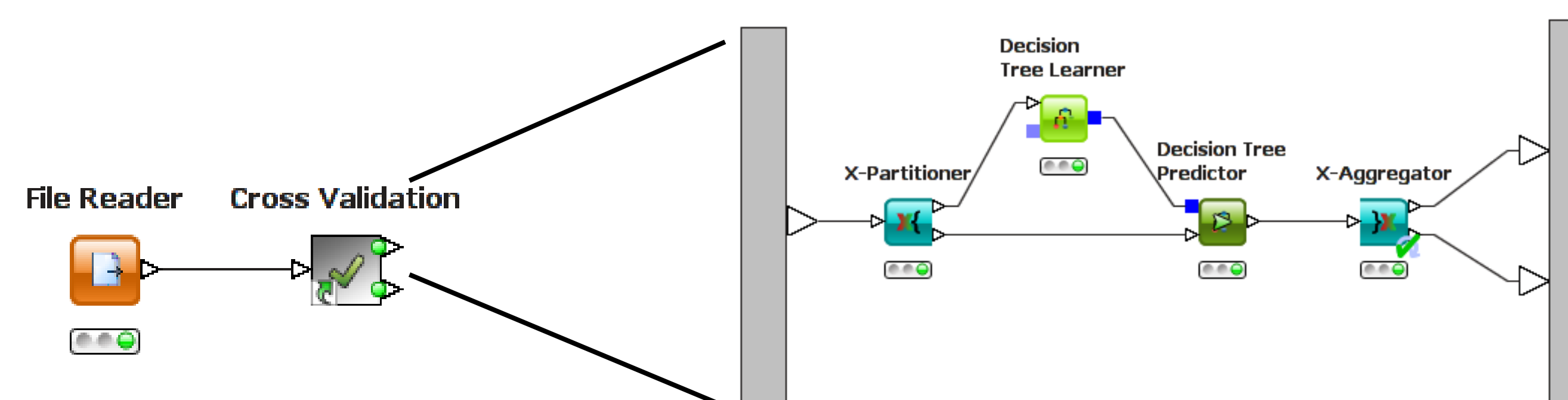
## KNIME WebPortal

- Access to workflows via a web browser
- Workflows can be executed on the server after login
  - Allows for user parameter input and file upload
  - Download results as CSV, PDF, DOC, ...



## Linked Metanodes

- Metanodes encapsulate sub-workflows which perform common tasks



- Metanodes can be saved as templates on a server and subsequently be like normal nodes
- Changes to the template on the server can be incorporated into the local workflow on demand

## Acknowledgements

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