



# The open integration platform

Chemaxon UGM Budapest, 20 May 2014

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KNIME.com AG

# Who is KNIME?

2004: KNIME development commences

2006: KNIME v1 released

2006: Spin-off in Konstanz, Germany

2006-2007: First commercial partners

2008: KNIME moves to Zurich

2010: Enterprise products released

2011: KNIME.com AG founded

2013: KNIME opens San Francisco office...

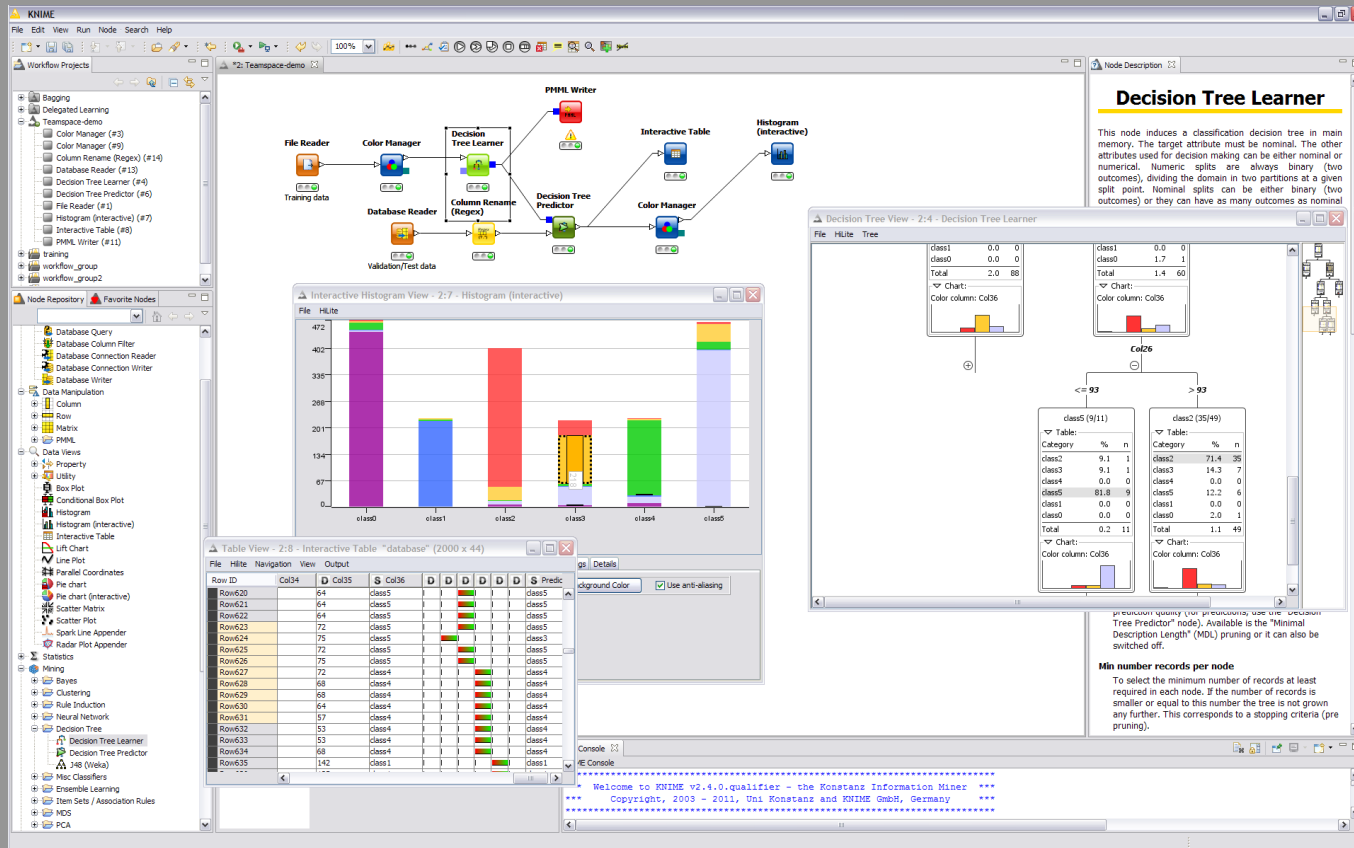
2014: KNIME opens Berlin office (May '14)



„KNIME saved my  
life in a world of scripts  
that I do not want to learn!“

2012

# The KNIME Platform



The screenshot displays the KNIME platform interface with a workflow titled "Teaspace-demo". The workflow includes nodes for File Reader, Color Manager, Database Reader, Decision Tree Learner, Column Rename (Regex), Decision Tree Predictor, Interactive Table, and Histogram (interactive). A PHML Writer node is also present.

The **Decision Tree Learner** node description is shown, explaining its function: "This node induces a classification decision tree in main memory. The target attribute must be nominal. The other attributes used for decision making can be either nominal or numerical. Numeric splits are always binary (two outcomes), dividing the domain in two partitions at a given split point. Nominal splits can be either binary (two outcomes) or they can have as many outcomes as nominal".

The **Decision Tree View - 2:4 - Decision Tree Learner** window displays the learned tree structure. The root node splits on Col36. The left branch (<= 93) splits on Col36, leading to a leaf node (class5) with 9/11 records. The right branch (> 93) splits on Col36, leading to a leaf node (class2) with 35/49 records. Each leaf node includes a table of class counts and a small histogram.

The **Interactive Histogram View - 2:7 - Histogram (interactive)** window shows a bar chart with six bars representing classes class0 through class5. The y-axis ranges from 0 to 472.

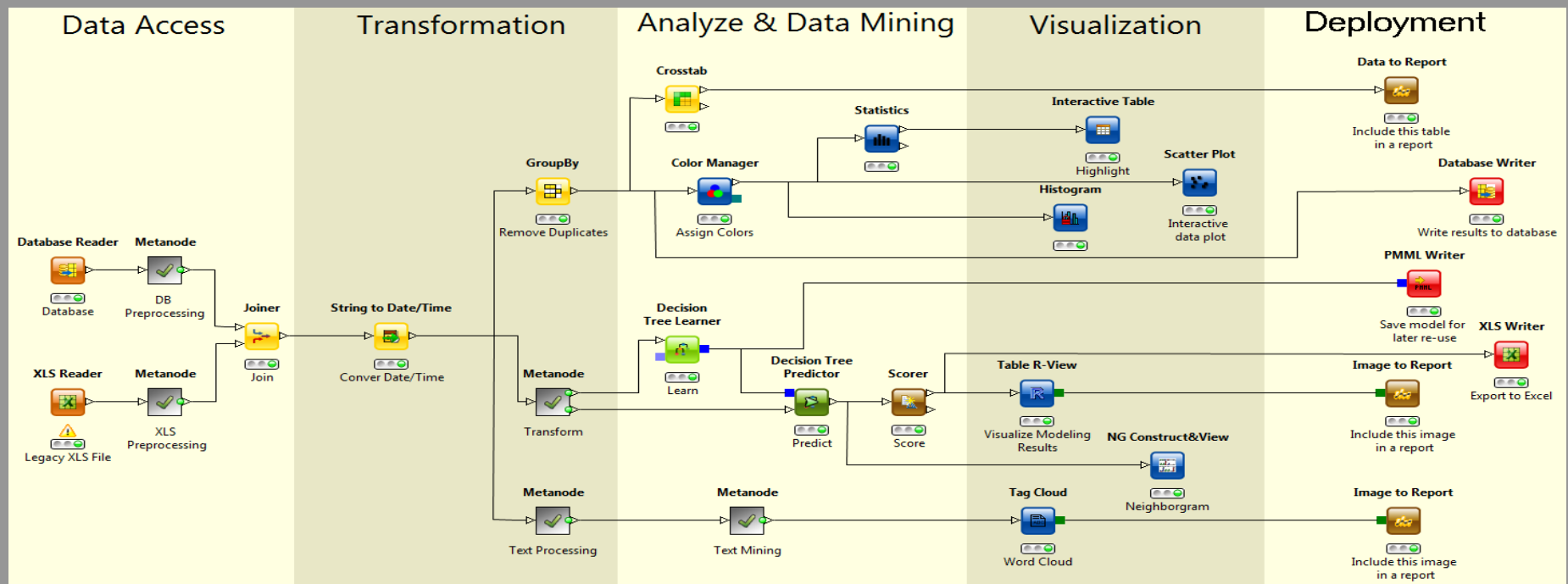
The **Table View - 2:8 - Interactive Table "database" (2000 x 44)** window shows a table with columns for Row ID, Col34, Col35, Col36, and Predict. The Predict column shows class assignments for each row.

The **Console** window at the bottom displays the following text:
 

```

    .....
    Welcome to KNIME v2.4.0.qualifier - the Konstanz Information Miner ***
    .....
    Copyright, 2005 - 2011, Ulf Koopman and KNIME GmbH, Germany
    .....
    
```

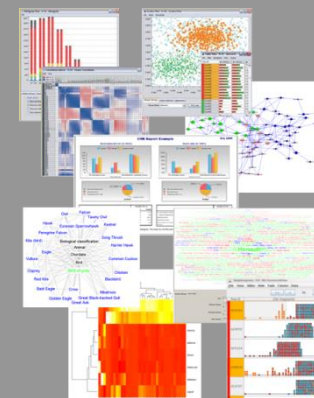
# Over 1000 native and embedded nodes included:



MySQL, Oracle, etc.  
 SAS, SPSS, etc.  
 Excel, Flat, etc.  
 Hive etc.  
 XML, PMML  
 Text, Doc, Image  
 Web Crawlers  
 Industry Specific  
 Community / 3rd

ETL  
 Row,  
 Column  
 Matrix  
 Text, Image  
 Time Series  
 Java  
 Python  
 Community / 3rd

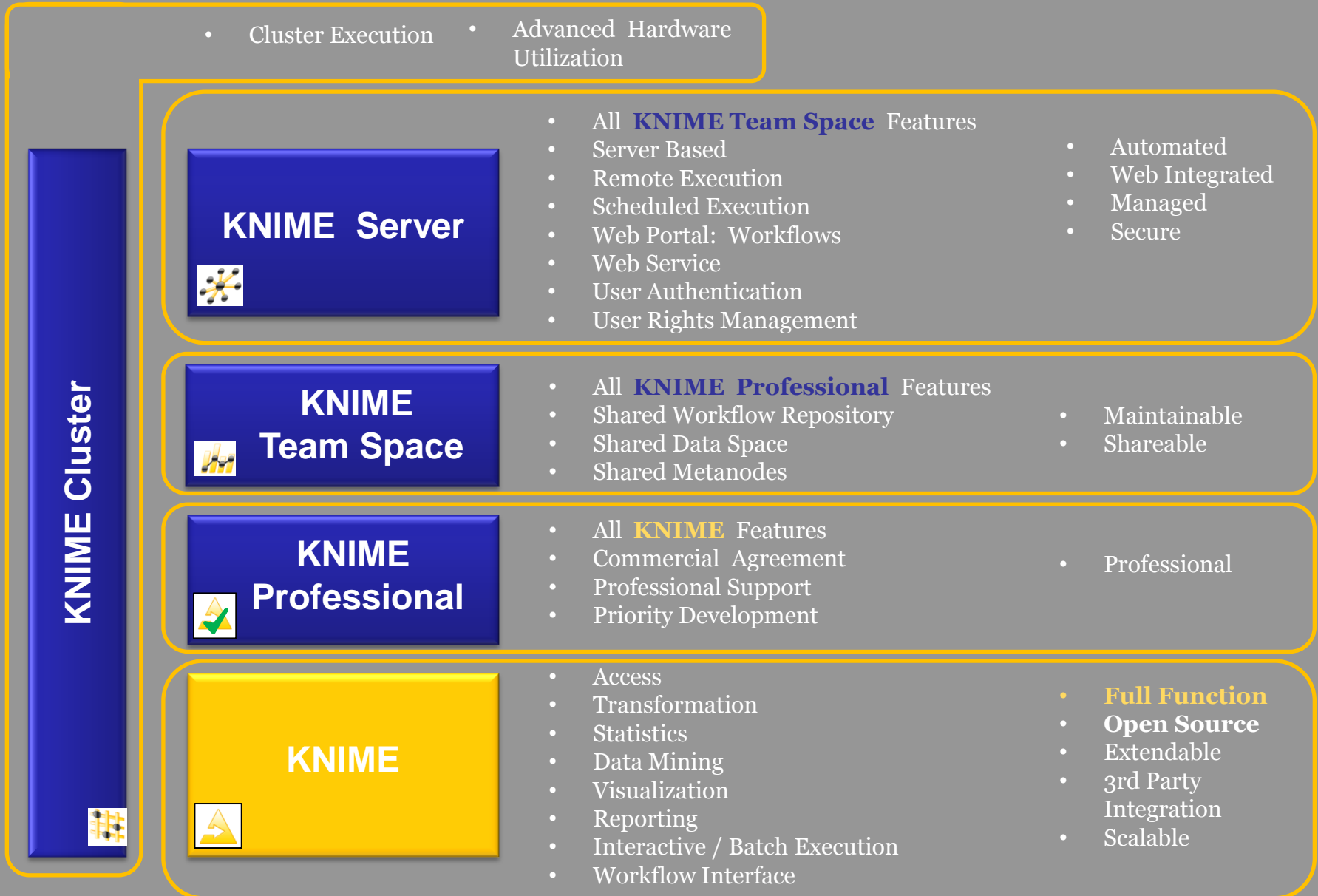
Statistics  
 Data Mining  
 Machine Learning  
 Web Analytics  
 Text Mining  
 Network Analysis  
 Social Media Analysis  
 WEKA  
 R  
 Community / 3rd



R  
 JFreeChart  
 Community / 3rd

via BIRT  
 PMML  
 XML  
 Databases  
 Excel, Flat, etc.  
 Hive etc.  
 Text, Doc, Image  
 Industry Specific  
 Community / 3rd

# KNIME Product Portfolio



# Technology Partner

- only Life Sciences -

- ChemAxon / Infocom
- CCG
- Schrödinger
- Cresset
- Tripos
- BioSolve IT
- Spotfire
- Molecular Discovery
- Trewaren
- Korilog
- Molegro



ChemAxon

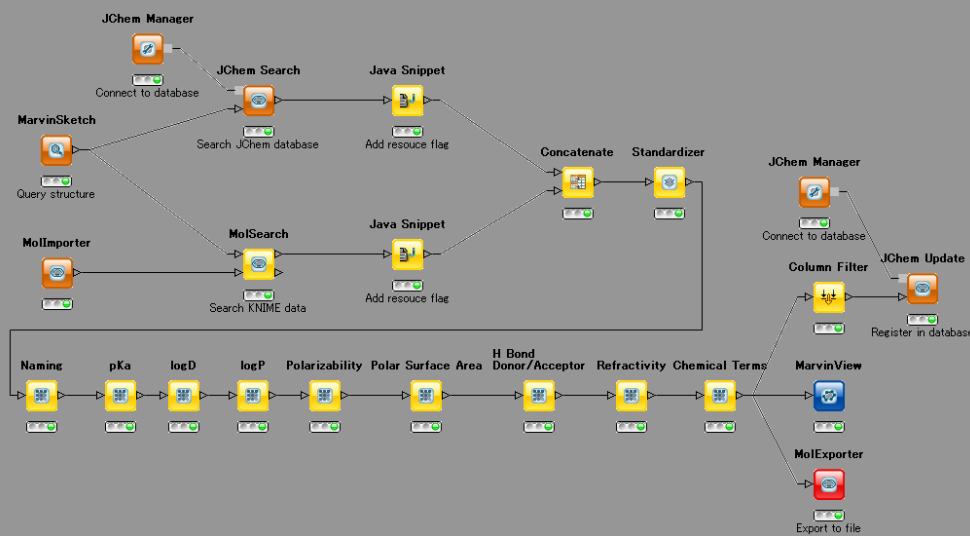
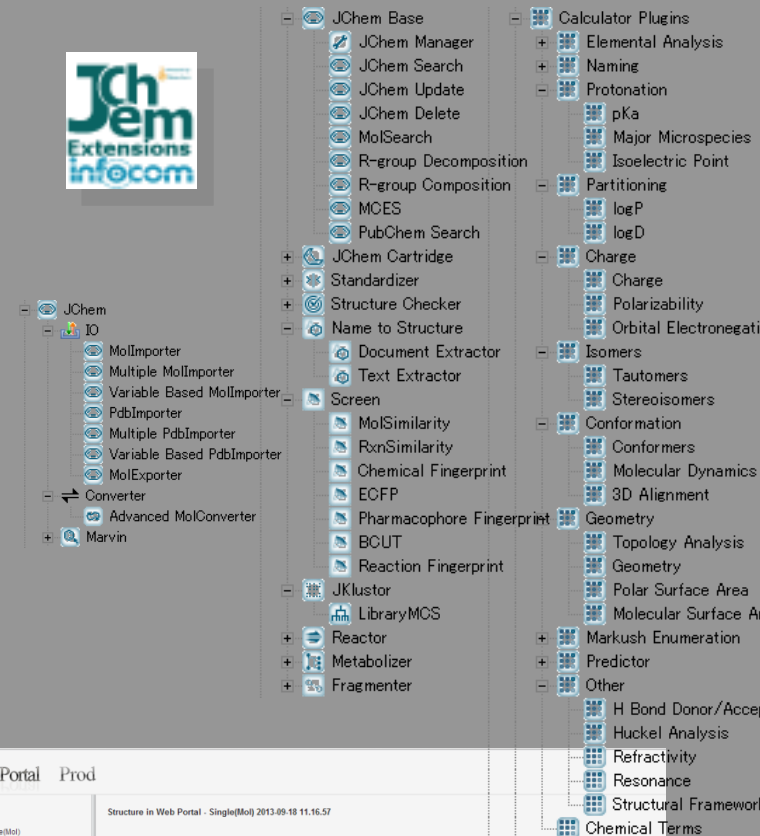
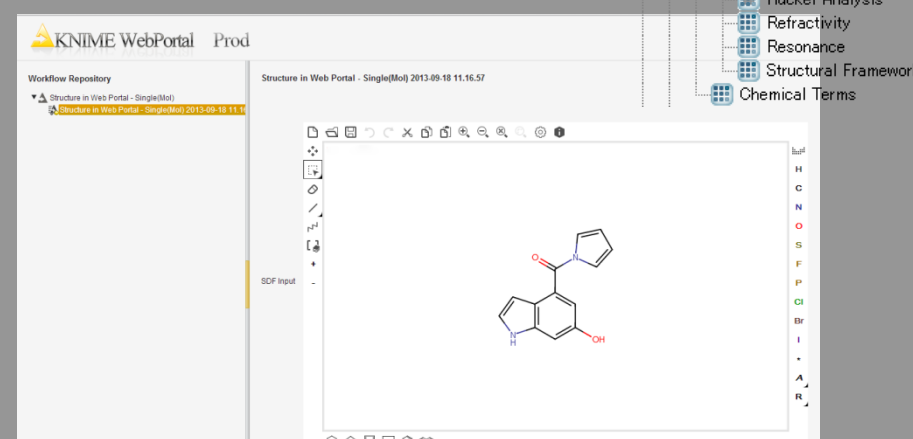


SCHRÖDINGER.



# JChem Extensions for KNIME

- Bring ChemAxon's cheminformatics to KNIME
- Developed by Infocom
- Majority of Jchem's cheminformatics tools
- MarvinJS for the Webportal

The screenshot shows the 'KNIME WebPortal Prod' interface. The 'Workflow Repository' on the left shows a workflow named 'Structure in Web Portal - Single(Mol)'. The main area displays the chemical structure of a molecule (SMILES: Oc1ccc(cc1C(=O)N2C=CC=C2)N3C=CC=CC3) and its analysis results. The 'SDF input' field is visible, and the 'Structure in Web Portal - Single(Mol) 2013-09-18 11:16:57' is shown. The right sidebar shows a legend for the chemical structure, including elements like H, C, N, O, S, F, P, Cl, Br, I, and A, R, L.

Thanks!