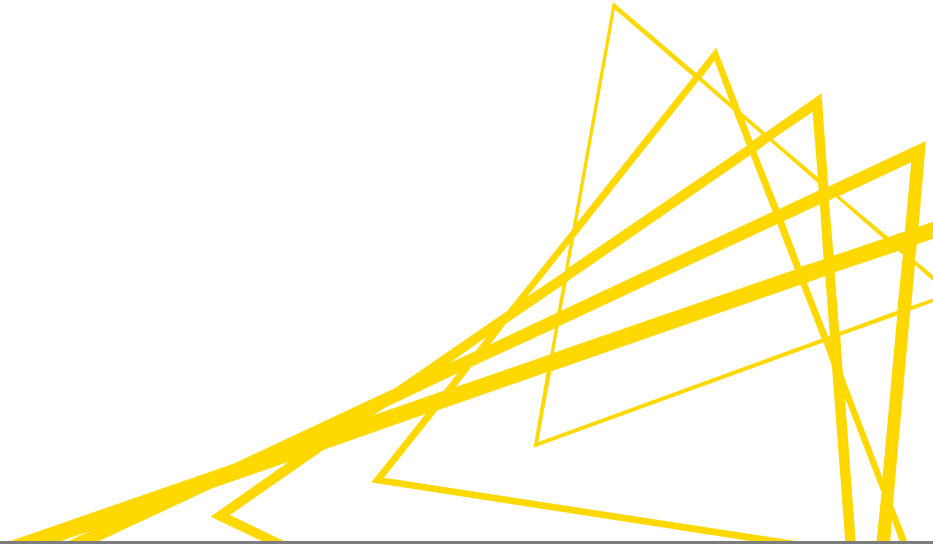




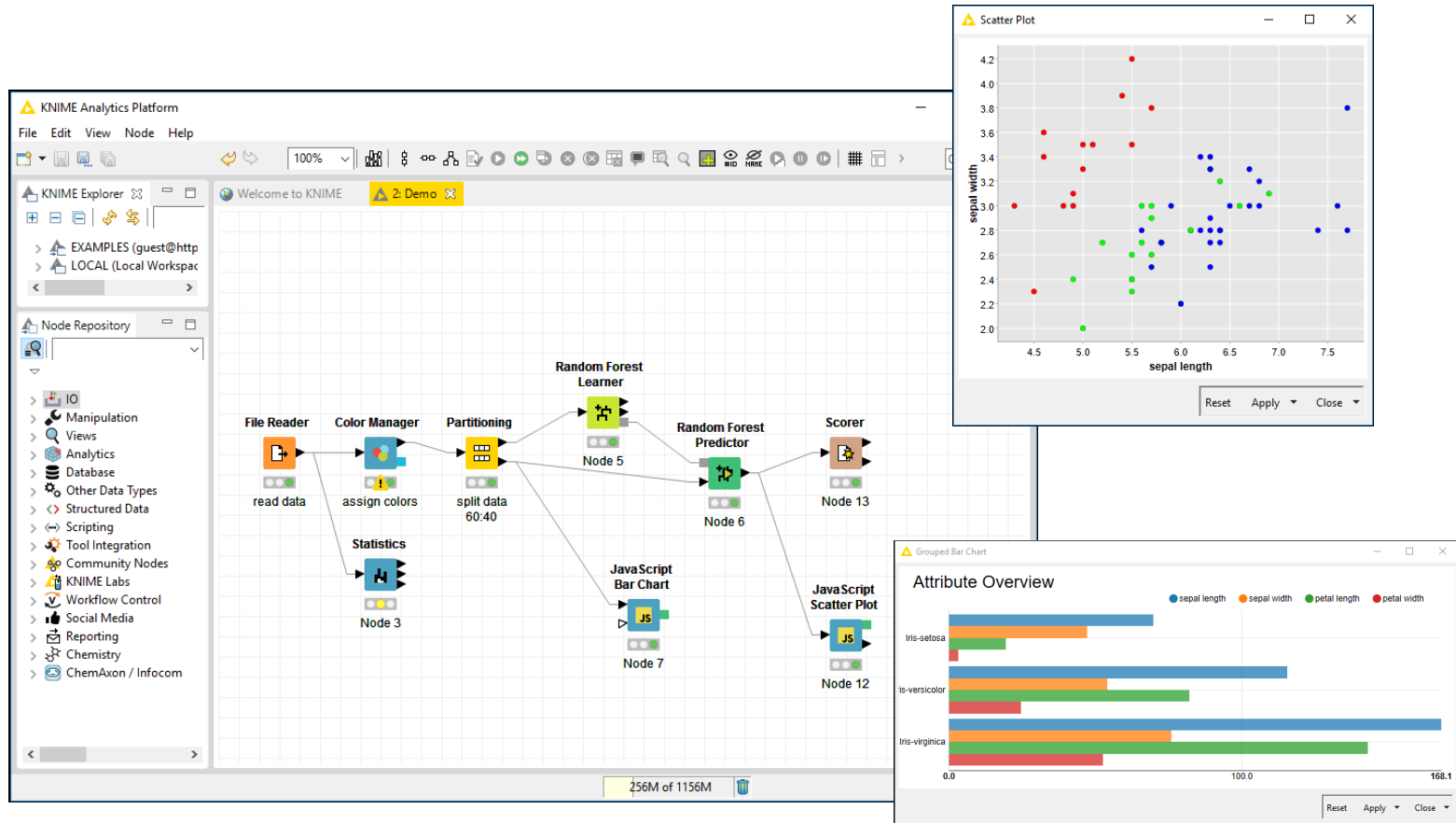
KNIME – ChemAxon Partner Presentation

Medzi
KNIME

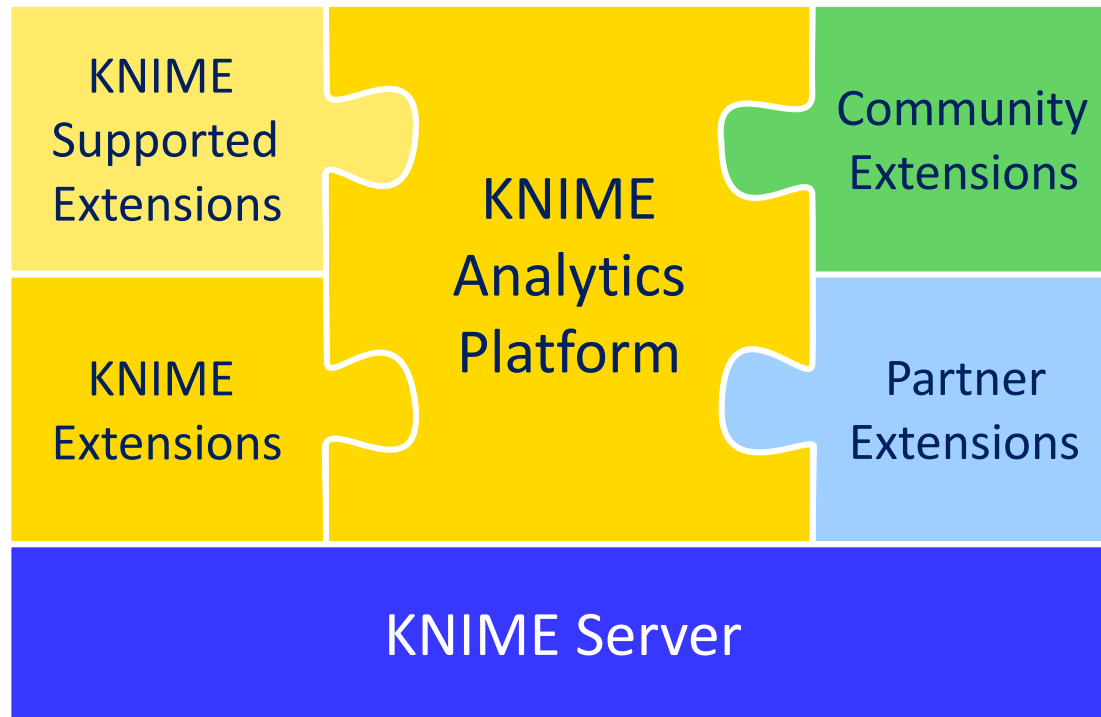
KNIME as an Open (Source) Platform



The KNIME[®] Analytics Platform



The KNIME Software Ecosystem



Collaboration:

- Compliance
- Best Practices
- Sharing Expertise

Automation:

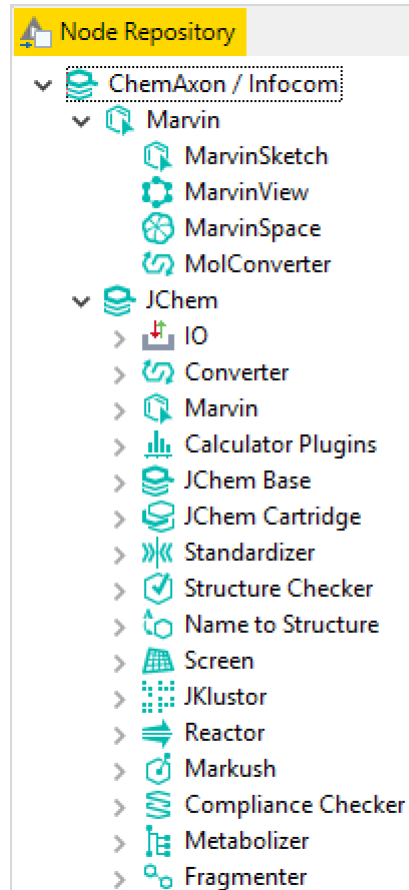
- Scheduling
- (Model) Management

Deployment:

- to Applications
- to Humans

ChemAxon/Infocom KNIME Nodes

- Several useful nodes donated to the Community – thanks!
- ChemAxon functionality available as KNIME nodes
- Mix and match that functionality with other technologies and techniques
- MarvinJS in KNIME Server WebPortal



The new KNIME Forum




























SOFTWARE / SOLUTIONS / LEARNING / PARTNERS / COMMUNITY / ABOUT















Log In  

You are here: Home / Community / Forum

https://forum.knime.com  Search

all categories  **Categories** Latest Top

Category	Topics
KNIME Analytics Platform For discussions related to KNIME Analytics Platform  General  Development	79 / month
KNIME Extensions For discussions related to KNIME Extensions  General  Text Processing  Scripting  Reporting  Image Processing  REST  BigData	19 / month
Community Extensions For discussions related to extensions developed by the KNIME community  General  RDKit  Scripting Extensions  Indigo  Ertwood  HCS Tools  Palladian & Selenium  CDK  OpenMS  Vernalis  Seqan	5 / month
Partner Extensions For discussions related to extensions developed by our KNIME partners  General  JChem Extensions  Schrödinger Extensions	65
Special Interest Groups For discussions related to various special interest groups  Cheminformatics  Bioinformatics	1 / month

Latest	
 Welcome to the new KNIME forum  KNIME Analytics Platform forum, website	1 1m
 KNIME Spring Summit 2018	2 Jan 24
 Welcome to Discourse	0 Dec '17
 How to merge images in different rows?  Image Processing	2 1d
 variable columns to 1 columns regularly  General	1 1d
 Cores used by Knime Cloud Analytics Platform  General	0 1d
 Waiting Too Long While Fetching 100 Rows Data from Database  General	0 1d
 Which Image Nodes already use multiple cores?  Image Processing	2 1d

Monster Model Factory

Monster model factory

/ˈmɒnstə mɒd(ə)l fækt(ə)ri/

noun

1. A tool for automating the process of building, validating, and deploying a daunting number of predictive models using KNIME

Overview

Init

Load

Transform

Learn

Score

Evaluate

Deploy

- Identified >1500 datasets from ChEMBL
- Created workflows for:
 - automating dataset extraction from the database
 - generating features for a dataset
 - automated model building and validation
 - deploying models that pass validation
- Automate the execution of that using the Model Factory
- Deployed models to KNIME Server as:
 - WebPortal application for model details
 - A REST service to generate predictions
 - WebPortal application for viewing predictions

Model Report for Assay: ChEMBL1212560

Confusion Matrix

		Predicted		
		active	inactive	
Real	active	11	1	0.92
	inactive	3	113	0.97
		0.79	0.99	

Performance:

AUC: 0.953

Enrichment factor at 1%, 5%, 10%: 8.333, 6.667, 7.500

Balanced Accuracy: 0.945

Cohen's kappa: 0.829

F-Score: 0.846

Assay Details

Description: Antimicrobial activity against *Pseudomonas aeruginosa* ATCC 13525 by MTT assay

standard_type: MIC

actives: 58; **measured inactives:** 0; **synthetic inactives:** 116

Model Details

Fingerprints: ECFP4

Method: Random Forest

trees: 200; **depth:** 15; **min_leaf_size:** 3

More on the Monster Model Factory

- Slides:
 - <http://bit.ly/2FQz7ML>
 - <http://bit.ly/2GNCrW6>
- Videos:
 - <https://www.youtube.com/watch?v=AwjbB5TnADg>
 - <https://youtu.be/QfKorunYrhk>

Server-managed customizations



How do I
configure
Python?



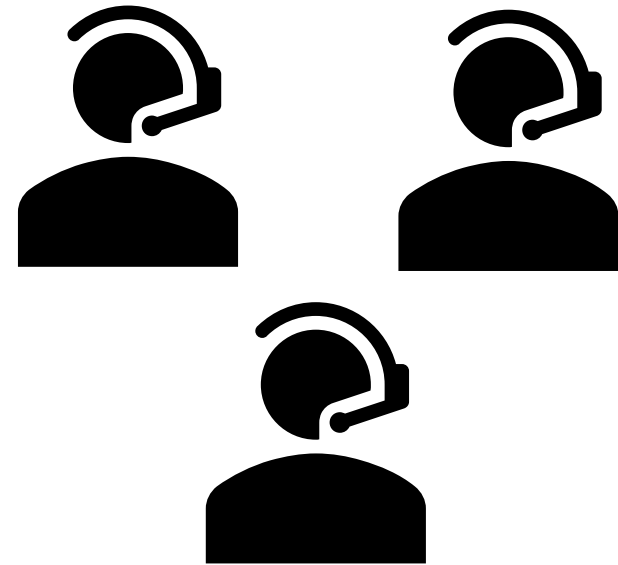
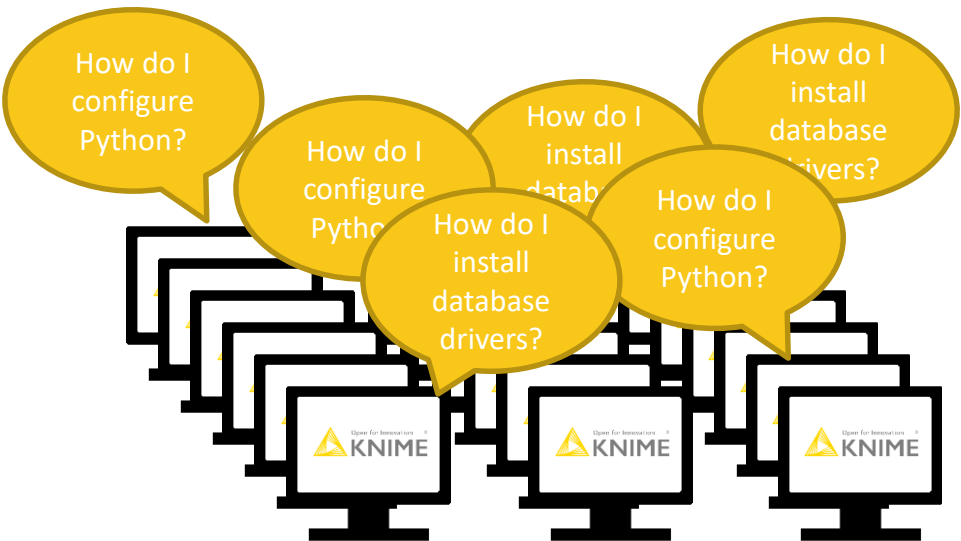
KNIME
Analytics
Platform

How do I
install
database
drivers?



KNIME
Analytics
Platform

Server-managed customizations



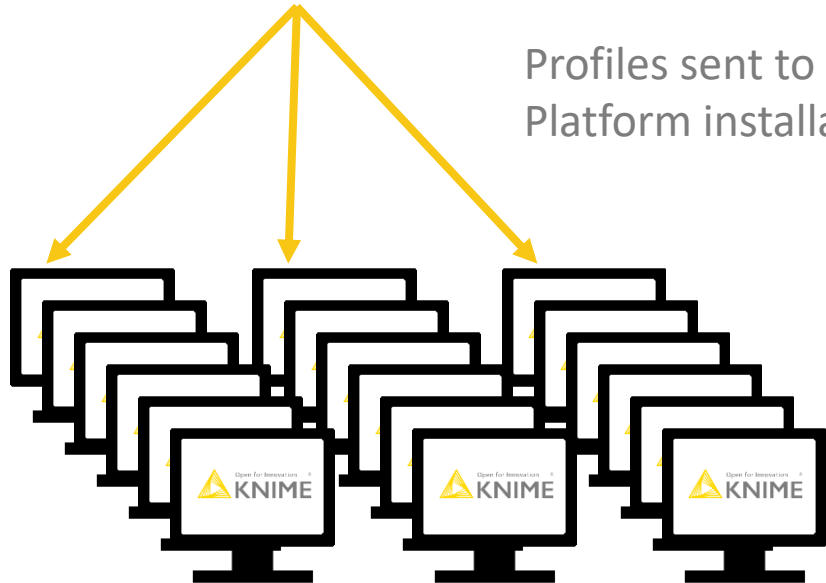
Server-managed customizations



KNIME Server

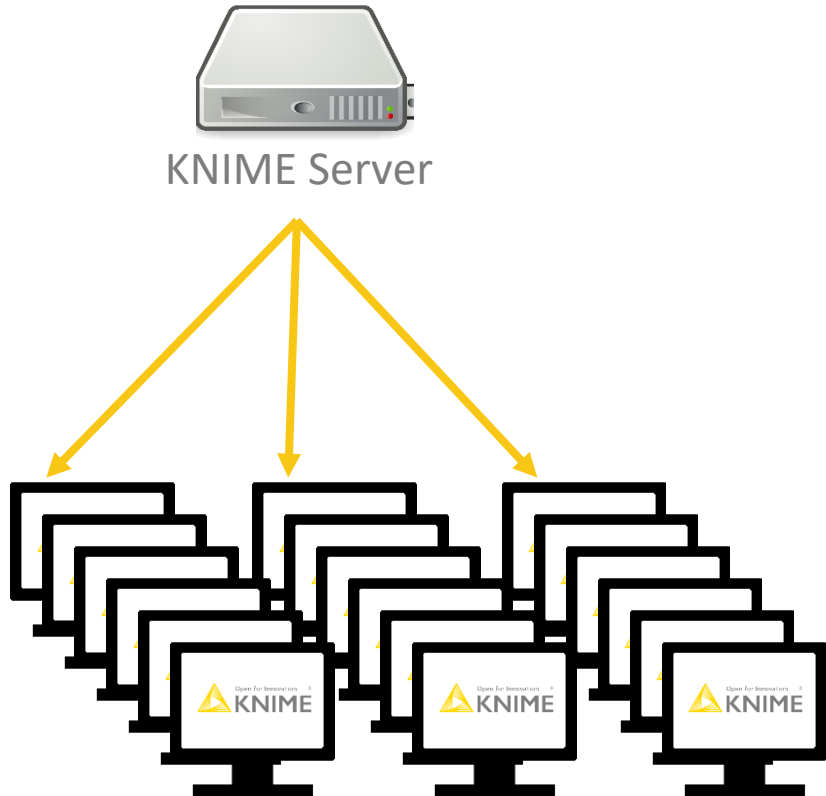


Profiles sent to Analytics Platform installations



Profiles can include:
Preferences, drivers, and more

Server-managed customizations



The screenshot shows the "Preferences" dialog box in KNIME, with the "Customization Profiles" section selected in the left sidebar. The main area contains the following content:

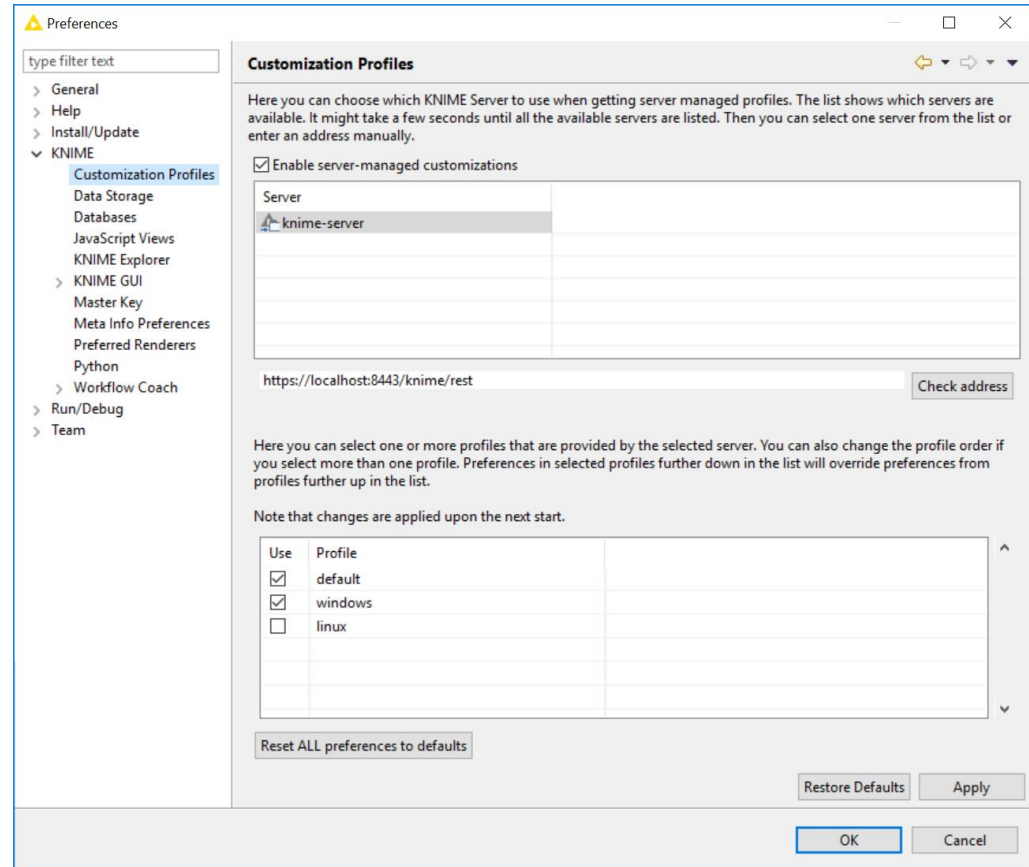
- Customization Profiles** (title bar)
- type filter text (input field)
- Navigation menu: > General, > Help, > Install/Update, > KNIME (expanded), > Customization Profiles (selected), > Data Storage, > Databases, > JavaScript Views, > KNIME Explorer, > KNIME GUI, > Master Key, > Meta Info Preferences, > Preferred Renderers, > Python, > Workflow Coach, > Run/Debug, > Team
- Customization Profiles** (section title)
- Text: "Here you can choose which KNIME Server to use when getting server managed profiles. The list shows which servers are available. It might take a few seconds until all the available servers are listed. Then you can select one server from the list or enter an address manually."
- Enable server-managed customizations
- Table with columns "Server" and "Address":

Server	Address
▲ knime-server	
- Text input field: `https://localhost:8443/knime/rest` with a "Check address" button.
- Text: "Here you can select one or more profiles that are provided by the selected server. You can also change the profile order if you select more than one profile. Preferences in selected profiles further down in the list will override preferences from profiles further up in the list."
- Text: "Note that changes are applied upon the next start."
- Table with columns "Use", "Profile", and "Address":

Use	Profile	Address
<input checked="" type="checkbox"/>	default	
<input checked="" type="checkbox"/>	windows	
<input type="checkbox"/>	linux	
- "Reset ALL preferences to defaults" button
- Buttons: "Restore Defaults", "Apply", "OK", "Cancel"

Server-managed customizations

- Profiles set on KNIME Server (can include e.g. Database JDBC drivers)
- Set in knime.ini to automatically pick up preferences
- Or manually set in preferences



KNIME is hiring!

- Software developers (Java and/or JavaScript)
- Data scientists (Application Scientists)
- Director of product marketing

Positions open in Austin, Berlin, Konstanz, and Zürich

More info: <https://www.knime.com/careers>

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