

ORAL PRESENTATION

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Get your chemistry right with KNIME

Thorsten Meinl^{1*}, Gregory Landrum²

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KNIME (Konstanz Information Miner, [1]) is a user-friendly and comprehensive open-source data integration, processing, analysis, and exploration platform. From day one, KNIME has been developed using rigorous software engineering practices and is used by professionals in both industry and academia in over 60 countries.

In the presentation we will show some of the new features in KNIME 2.6 and give an outlook to KNIME 2.7. We also present recent developments in the KNIME Community Contributions [2], where research groups can easily provide their KNIME extensions to the community. We will focus on the freely available chemistry extensions - especially RDKit [3] - and demonstrate their usage in real-world workflows.

Author details

¹University of Konstanz, Box 712, D-78457 Konstanz, Germany. ²Novartis Pharma AG, Postfach, CH-4002 Basel, Switzerland.

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References

1. [<http://www.knime.org/>].
2. [<http://tech.knime.org/community/>].
3. [<http://www.rdkit.org/>].

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* Correspondence: Thorsten.Meinl@uni-konstanz.de

¹University of Konstanz, Box 712, D-78457 Konstanz, Germany
Full list of author information is available at the end of the article