KNIME-CDK Updates

A Cheminformatics Extension for KNIME

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Chemistry Development Kit

An Open Source Java™ Library for Structural Chem- and Bioinformatics

- version 1.5.x → KNIME-CDK

Features

- reads and writes chemical data formats
- renders chemical structures
- substructure search and highlighting
- signature and fingerprint generation
- qsar descriptors
- …
- …
- …
- chemical graph theory

http://tech.knime.org/community/cdk
http://tech.knime.org/forum/cdk
CDK Evolution

Version 1.4.x  Version 1.5.x
Hydrogen Suppression
Substructure Search

SDF Reader → Substructure Search

Riboses

Molecules with fragment - 0:4 - Substructure Search

Row ID | Name | Molecule
--- | --- | ---
Row6 | 384279 | ![Molecule](molecule6)
Row7 | 393403 | ![Molecule](molecule7)
Row8 | 384282 | ![Molecule](molecule8)
Row9 | 393452 | ![Molecule](molecule9)
SMARTS
Partition Coefficients

- Reference Set: ~1600 compounds
- RMSE = 0.932
Tautomers

- AMBIT is an open source software for cheminformatics data management
  - Lesser General Public License version 2.1
  - Version 2.6.0-SNAPSHOT
  - http://ambit.sourceforge.net/

[Diagrams of AMBIT software interfaces showing tautomer generation and structural sketches.]
Nightly Build

Nightly builds
The Nightly builds update site needs to be added manually to the list of Available Update Sites (see above for instructions).

- [http://tech.knime.org/update/community-contributions/trunk](http://tech.knime.org/update/community-contributions/trunk) for the nightly builds or download a zipped update site. Note the the nightly build may require the latest KNIME version.

The newly installed nodes will appear in KNIME in a new category "Community Nodes".

*Please note that KNIME does not take any responsibility for the extensions provided by the community.*

- The changes very likely to cause regression in existing workflows!
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