

CDK Bug Squash Party - Day 3 and 4

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Citation

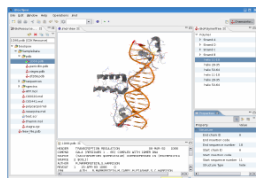
Willighagen, E. (2006, September 22). CDK Bug Squash Party - Day 3 and 4. *Chem-bla-ics*. <https://doi.org/10.59350/zwkym-aty79>

Keywords

Cdk, Bsp, Java, Pdb, Conference

Bioclipse

Bioclipse is an Eclipse-based result viewer which allows the editing and viewing of chemical and biological data. It features small molecules, proteins, RNA, DNA, sequences, alignments and spectra's



Scripting Languages

Allows writing short pieces of customized functionality.

- Ruby
- Python
- BeanShell (Java)

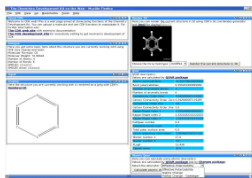
Ruby

```
parser = SmilesParser.new
smiles = 'Clc1ccccc1'
mol = parser.parseSmiles(smiles)
puts mol.getAtomCount
```

Database / Websites

Integration with databases and websites

- Java Servlets / Ruby on Rails
- SQL via JDBC
- Ruby on Rails
- webservices

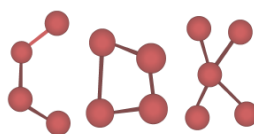


More information

- <http://cdk.sourceforge.net>
- <http://www.chemistry-development-kit.org/>
- <http://cdk.sourceforge.net/wiki>
- cdk-user@lists.sourceforge.net

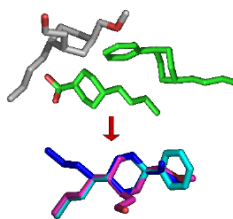
Steinbeck, C., Han, Y., Kuhn, S., Hellerich, O., Luttmann, E. and Willighagen, E. The Chemistry Development Kit (CDK): An Open-Source Java Library for Chemo- and Bioinformatics. *Journal of Chemical Information and Computer Sciences* 2003, 43, 493-500.

Steinbeck, C., Hoppe, C., Fuhn, S., Guba, R., Willighagen, E. L. Recent Developments of The Chemistry Development Kit (CDK) - An Open-Source Java Library for Chemo- and Bioinformatics. *Current Pharmaceutical Design* 2006, 12, 2111-2130.



The Chemistry Development Kit

<http://cdk.sf.net/>



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