

chem-bla-ics

Open Infrastructures #1: Research Software Directory

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Keywords

Cdk, Openscience

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| *Research software is an integral part of scientific investigations.*

This is what Struck wrote in 2018 in a contribution to the 2018 IEEE 14th International Conference on e-Science (e-Science) (doi:[10.1109/eScience.2018.00016](https://doi.org/10.1109/eScience.2018.00016)). I very much agree with this, and the notion is gaining ground in the academic community. Their paper "*identifies challenges, risks and new opportunities in research software publication and discovery*".

At the same conference, Spaaks *et al.* presented a lightning talk about the [Research Software Directory](#) (RSD), "*a content management system for research software, which promotes the visibility, reuse, and impact of research software*" (doi:[10.1109/eScience.2018.00013](https://doi.org/10.1109/eScience.2018.00013)).

I wonder who spoke first at the meeting.

Anyway, I learned about RSD a while ago already and have been using it for some of our group's research software. We don't have a collection for our group, but you will find them under the [Maastricht University organisation page](#).

And as sketched by Struck and implemented by Spaaks *et al.*, RSD gives rich context to the research software. It can track the activity on the project (for GitHub, GitLab, [Codeberg](#) etc), track citations to key literature, and can have links to distributions where the software is published (like Debian, CRAN, [Bioconductor](#), etc).

This is what it looks like for the [Chemistry Development Kit](#):

Chemistry Development Kit

1793 5

mentions contributors

Open Source cheminformatics library.

Get started ↔



7236 commits | Last commit ~ 1 week ago | 559 stars | 173 forks

Cite this software

DOI:

10.5281/zenodo.15105090



Copy DOI

Software version:

cdk-2.11

Choose a reference manager format:

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Description

The Chemistry Development Kit is a Java library with cheminformatics functionality. It can read many chemistry file formats (MDL molfile and SD file, XYZ, PDB, etc), line notations (SMILES), produce InChI, calculate molecular descriptors, depict chemical structures as 2D SVG, and a lot more.



Keywords

Cheminformatics

Chemistry

Computational Chemistry

Programming language

Java 100%

License

LGPL-2.1-or-later

Source code



Packages



I like initiatives like this, as they help the community work out open standards to exchange metadata, and encourage other projects by reusing their APIs.