

chem-bla-ics

# CDK 2.12

Egon Willighagen 

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## Keywords

Cdk, Openscience

## Abstract

Version 2.12 of the Chemistry Development Kit has been released. It is the last release with contributions by our NWO Open Science grant.

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## chem-bla-ics

Version 2.12 of the [Chemistry Development Kit](#) has been released. It is the last release with contributions by [our NWO Open Science grant](#). This release adds some nice new APIs:

- harmonize hydrogens to various states: depiction, stereo, minimal, and unsafe (useful for depictions)
- generate wedge bonds based on coordinates and stereochemistry
- more Markush / RGroup support
- atropisomers via CXSMILES
- sugar extraction

I also update the following libraries/tools to use CDK 2.12:

- [NanoJava 2.16](#)
- [Bacting 1.0.10](#) (and the Python pyBacting will follow asap)