

chem-bla-ics

CDK 2.12

Egon Willighagen 

Published March 8, 2026

Citation

Willighagen, E. (2026). CDK 2.12. In *chem-bla-ics*. chem-bla-ics. <https://doi.org/10.59350/gw9at-srp84>

Keywords

Cdk, Openscience

Copyright

Copyright © Egon Willighagen 2026. Distributed under the terms of the [Creative Commons Attribution 4.0 International License](#), which permits unrestricted use, distribution, and reproduction in any medium, provided the original author and source are credited.

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)