

cdk2024 #5: Chemistry Development Kit User Group Meeting - Day 2

Egon Willighagen 

Published March 16, 2025

Citation

Willighagen, E. (2025, March 16). cdk2024 #5: Chemistry Development Kit User Group Meeting - Day 2. *Chem-bla-ics*. <https://doi.org/10.59350/n7e6r-p1e93>

Keywords

Cdk, Openscience, Cdk2024

Abstract

Where the first workshop day had several talks about new and old features of the Chemistry Development Kit (CDK), the second day was a hackathon day. We hacked and we talked.

Copyright

Copyright © Egon Willighagen 2025. 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.

Where [the first workshop day](#) had several talks about new and old features of the [Chemistry Development Kit](#) (CDK), the second day was a hackathon day. We hacked and we talked. The coding was not mostly only the CDK repository itself, but [some things happened there](#) too:

main	All users	All time
Commits on Mar 11, 2025		
Catch the Factory configuration exception in SAX johnmay authored and egonw committed 5 days ago · ✖ 8 / 9	f8621e5	
Remaining JavaDoc errors fixed johnmay committed 5 days ago · ✓ 9 / 9	3ee4874	
Merge pull request #1168 from Mailaender/javadoc-cleanup johnmay authored 5 days ago · ✓ 9 / 9	Verified 6e32a6b	
Fix JavaDoc warnings. Mailaender committed 5 days ago · ✖ 6 / 7	7263da0	
New year egonw authored 5 days ago · ✓ 7 / 7	Verified c0378cf	
New link egonw authored 5 days ago · ✓ 7 / 7	Verified fd1ecce	
Merge pull request #1166 from cdk/remove/profilerAck johnmay authored 5 days ago · ✓ 7 / 7	Verified 83bf0fc	
The free (for OS projects) license hasn't been used for some time now egonw authored 5 days ago · ✓ 9 / 9	Verified c670ff9	

Some pointers:

- we worked on the [Groovy Cheminformatics with the Chemistry Development Kit](#) book
 - move the repository to the GitHub organisation
 - improved the build system
- it was explored how the CDK can generate SMILES for glycans
- continued work on updated tools using the CDK, e.g. [ChemViz2](#)
- code clean up, e.g. on [JavaDoc](#) and [the XML parsing](#)
- a [JChemPaint release, based on CDK 2.10](#), with a [flatpak for easy install on many Linux distributions](#)

We further had discussions about a possible change of the license (what it would involve) and OSGi support. The problem there is that Java packages can only exist in one OSGi bundle, and this is currently not the discuss. We discussed that the current modules were partially setup to clean up dependencies, and generally modularize the CDK (e.g. each module could have a separate person responsible). We now want to propose a larger **core** module which covers the common cheminformatics functionality. A final discussion point I want to mention is that there are serious hints that we may have the Chemistry Development Kit as JavaScript in the browser soon!

chem-bla-ics

I like to thank every one who joined the workshop, particularly those that travelled to Maastricht from the UK, Germany, and Bulgaria. Also thanks to the six participants online who joined on the first day!