

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

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Published March 16, 2025

Citation

Willighagen, E. (2025). cdk2024 #5: Chemistry Development Kit User Group Meeting - Day 2. In *chem-bla-ics*. 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.

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chem-bla-ics

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:

The screenshot shows a list of commits on the GitHub interface for the 'chem-bla-ics' repository. At the top, there are filters for 'main' branch, 'All users', and 'All time'. Below the filters, the commit history for 'Commits on Mar 11, 2025' is displayed. Each commit entry includes a title, author information, a commit hash, and a 'Verified' badge. The commits are as follows:

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

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!

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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!