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

Egon Willighagen ⓘ

Citation

Keywords

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

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:

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!