CDK 1.0: a milestone after 7 year of development

Egon Willighagen ⓘD

Citation

Keywords

Copyright

chem-bla-ics

Last night, I released CDK 1.0 as the previous release candidate did not show up new major problems. It is far from a perfect release (see these still TODO's and Nightly, run by Rajarshi), but the core is pretty solid.

I would warmly thank everyone who has contributed to the project in one way or another (I worked more on maintainance than implementing functionality), as it has been a great pleasure to make CDK releases. OHLOH runs a rather nice developer hall of fame for the CDK. You'll see that Christoph's research group is the major contributor. User contributions, however, are equally important and played a bug role in the quite large set of JUnit tests we have now (3300+).

Another reason why this is an important milestone, is that it is the last release I am creating. I wrote on the user list:

> • *In advance of the actual CDK 1.0 release, thanx very much to all that contributed big *and* small ! It was a great 7 years of open source chemoinformatics development! Hey, that actually sounds like I am stepping down... Well, it *is* time for a new generation to step up indeed. I won't leave the project, but being CDK News editor, CDK release manager, CDK code developer is a bit much for doing outside office hours. I feel that I have clearly enough made my point for open source chemoinformatics, and it is time for something else... which will very likely involve the CDK, but likely more as user only... I was hoping in the past few years, that the transition would go smoothly, and have been trying to get people interested in various emails, including this one; however, being humans, we wait for the catastrophe and only after that we're shocked and start doing something about it. So, yeah, I'm forced to make this drastic announcement: CDK 1.0 will be the last CDK release *I* will make.*

So, who wants to take over? Some one will have to. I, however, will put my focus on other things. Very likely involving the CDK, as there are still many things I want to do. Some things I have on my list:

- the Java2D based 2D renderer/editor
- more accurate atom type perception
- more articles for CDK News
- the book "CDK for Dummies"
- improved structure generator
- validation
- ...