chem-bla-ics

CDK 1.0: a milestone after 7 year of development



Published April 23, 2007

Citation

Willighagen, E. (2007, April 23). CDK 1.0: a milestone after 7 year of development. *Chem-bla-ics*. https://doi.org/10.59350/qd21w-71g30

Keywords

Cdk, Cheminf, Junit

Abstract

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.

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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

• ...