

chem-bla-ics

CDK 1.2 Release Candidate

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I released [CDK 1.1.5](#) today. Below is the email I sent to the [cdk-user mailing list](#):

Hi all,

I am happy to be able to announce the first Release Candidate for CDK 1.2.

Everyone using using CDK 1.0 is suggest to upgrade to this release, which has fewer bugs, is much better tested, and is faster too. It also comes with API changes, and a full changelog is not available (yet). However, the CDK developers are available on this mailing list and on IRC to help you port CDK 1.0 applications to CDK 1.2. Two differences in particular I would like to point out at this moment:

1. explicit atom typing

CDK 1.0 did atom typing at various places to perform its function, leading to inconsistencies and bugs. CDK 1.2 introduces a new atom typing module which isolates atom typing from other algorithms. Consequently, the CDK will be more critical on your code and your data: where the old code might have silently eaten incorrect input, the new implementation complains: expect exceptions! The actual atom type list used in CDK 1.2 is more complete than the ones used in CDK 1.0; however, it is not unlikely that you will find no atom type perceived for a clearly valid atom type. Please report such cases.

And I really want to stress this: in every instance where CDK 1.2, CDK 1.0 would have failed too, though it might have not complained about it.

2. no rendering functionality

The new rendered under development (see the [cdk-jchempaint mailing list](#)) has not made the CDK 1.2.0 release. However, it is expected to be available in a later CDK 1.2.x release. If you really need the graphics functionality, please contact me. Bioclipse2 is an example project which combines CDK 1.2 with the new rendering code.

Contributions

This release features contributions from a larger developer group than ever before. In particular, I would like to welcome those who have picked up JuniorJobs, and provided other smaller patches! A full list of authors is available from:

<http://cdk.svn.sourceforge.net/viewvc/cdk/cdk/tags/cdk-1.1.5/AUTHORS>

(If you see your name missing (sorry!), please just email me)

If you like to contribute too, there are many ways. The JuniorJobs is just an example and are available from:

http://sourceforge.net/tracker/?group_id=20024&atid=997721

Download

CDK 1.2 RC1 is available from SourceForge as CDK 1.1.5:

http://sourceforge.net/project/showfiles.php?group_id=20024&package_id=57806

Alternatively, you can download the release from SVN:

<http://cdk.svn.sourceforge.net/viewvc/cdk/cdk/tags/cdk-1.1.5/>

Bugs

As said, this CDK release is the most tested CDK release ever, with more than 10 thousand unit tests! However, there are open (minor) issues, which you can see reported at Nightly:

<http://pele.farmbio.uu.se/nightly-1.2.x/>

The number of failing unit tests is below 1%, and in the same range as the number of failing tests for CDK 1.0. Importantly, these are typically fails of unit tests which are not available in the CDK 1.0 unit test suite; that is, many of the failing unit tests in CDK 1.0 are not failing in CDK 1.2 (it really is rewarding to upgrade!)

However, if you find additional bugs (or just have wishlists), you can report these with our SourceForge bug tracker at:

http://sourceforge.net/tracker/?group_id=20024&atid=120024

Documentation

Over the next weeks I hope to compose a somewhat useful list of changes. I have not made up my mind yet how that will take shape, maybe as a list of blogs, which I'll aggregate later. Dunno yet. Suggestions and contributions welcome :)

JavaDoc for the release is not yet available on SF for download (working on that), but available for the cdk1.2.x / branch at:

<http://pele.farmbio.uu.se/nightly-1.2.x/api/>

OK, that wraps it up for now. Just reply if you have questions.

Egon