

chem-bla-ics

CDK 1.2.1 Released

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Keywords

Cdk

Abstract

I just released CDK 1.2.1 (aka The CDK Workshop 2009 Release), which is now available for download from SourceForge. The source can be found in our Git repository.

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chem-bla-ics

I just released [CDK 1.2.1](#) (aka *The CDK Workshop 2009 Release*), which is now available for [download from SourceForge](#). The source can be found in [our Git repository](#). The changes since 1.2.0 are mostly bug fixing, new unit tests, and minor clean up here and there:

Fixed bug 2714283, which properly throws an exception when rings are not closed properly.
Fixed bug 2729120 and added unit test
Updated comment to fix bug 2768643.
Partial fix for bug 2719237. Made getBondOrderSum static, added unit test for it
Typo: proteinl -> protein
Made class public, to unbreak adding it to the build/*.javafiles
Partially fixed SMARTS matching for R0. Updated target molecule initialization to explicit
Fixed dubious equality test. A private method was checking Double objects via reference.
Added test method annotation. Completes coverage for data module
Refactored ChiIndexUtils to make it package private. Cleans up public API, since it is on
Code cleanup of ChiIndexUtils. Converted to 1.5 idioms
Clean up of PathTools and added test method annotation, so that core is completely covered
Fixed the previous commit to edit the cdk.keyword line, not the cdk.module line
More consistent keywords used
Added a test to ensure that Integer objects are compared by value rather than reference
Added a test case to check that atom container diffs are correct when using deserialized
Fixed IntegerDifference so that it actually checks the integer value rather than reference
Applied patch #2675819 (Stefan Kuhn): Patch to add a removeReaction to reactionSet
Use interface instead of implementation
Removed an unused import
Use IAtomContainer instead of IMolecule, as the actual matching is using IAtomContainers
Fixed a ClassCastException (fixes #2685134)
Added source attrib to fix building the Ubuntu .deb
Fixed Help build system: use doclet jars in develjar/; updated for new src folder src/main
Removed libdepends include for test-ioformats, which does not actually have libdepends
Updated so that if a target atom has no symbol (such as pseudo atoms) the match returns false
Fixed proper handling of #n SMARTS queries
Added test case for bug 2686473
Added note on Ant 1.7.1 required
Fixed a NPE source: 'null == 2' causes an exception, so first test for nullness
Fixed copyright notice for 2009
Fixed duplicate storage of layout templates, which only belong in the sdg module, not ext
Merge branch 'local1.2' of ../../git-svn/cdk

Thank you for all who reported bug reports!