chem-bla-ics

CDK 1.3.1: the changes

Egon Willighagen

Published December 2, 2009

Citation
Willighagen, E. (n.d.). In *chem-bla-ics*. chem-bla-ics. https://doi.org/10.59350/m46g1-09v92

Keywords
Cdk, Git

Copyright
Copyright © Egon Willighagen 2009. Distributed under the terms of the Creative Commons Attribution 4.0 International License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original author and source are credited.

Two weeks ago, I released CDK 1.2.4. Anay reported fails with generating the JavaDoc from the packages, which I think I both fixed now; the uploaded 1.2.4.1 packages on SourceForge include these fixes.

The 1.2.4 release was soon followed by 1.3.1. Unfortunately, uploading the packages to to SourceForge over 3G with Chrome did not work well, so only finished that today. CDK 1.3.1 is the second release in the development branch, and brings in new functionality but also API changes. Here are the changes since the 1.3.0 release:

- Bumped version for 1.3.1 release c34109572d
- Added some extra lines, hopefully fixing the conflicts all the time 6dab943dd2
- Merged changes from the CDK 1.2.4 release c31c297a59
- Fixed param name 743bad345e
- Updated the makefp3d target to work with the current build system bbb78ee581
- Set up a branch for the 1.2.4 release 4801d79b8c
- Fixes bug 2898399. Updates to the SMARTS parser to handle proper matching for explicit hydrogens (including H, 1H, 2H and 3H). SMARTSQueryVisitor updated to take into account different isotopes of H. Also updated unit tests to take into account proper H matching. Added a unit test to further check H matching. b67d76ac96
- Added tests to match hydrogens 45a7f54c3d
- Fixed junior issue 1816529: Missing Java5 generics for atomContainers() Iterator 484619e35d
- Reworked the tests for bug 2898032. Updated Javadocs for smiles generator 7f68b07aa8
- Added unit test to confirm and check for bug 2898032 924b56395e
- Fixed junior issue 1802586: Misuse of assertTrue for tested strings 12bec4f992
- Made the AtomContainerPermutors IAtomContainer implementation independent 4748098973
- Merge branch 'cdk-1.2.x' 8a95d93506
- Updated UIT to handle single atom queries and added a unit test for bug 2888845. Also updated Javadocs to specifically note behavior of single atom queries dfb28054f2
- Fixed the dist-large target: removed to no longer existing .libdepends after the log4j module patch 9dc13e3c33
- Implemented instantiating custom loggers; example in the unit test class 2771eb94db
- Added the use of the SystemOutLoggingTool as back up acf59538e9
- Added a ILoggerTool implementation for STDOUT 921447a690
- Dig up and updated the copyright history a3cc8764b6
- Factored out initialization of the tool, to allow reusing the code for other logger class names 2af5f247fb
- Moved the log4j.jar depending LoggingTool into a separate module 112f64d6a0
- Introduces the ILoggingTool interface and a factory so that CDK code no longer needs to depend on LoggingTool which depends on Apache's Log4j library. c6c8d38a93
- Added generation of java source jars e33fba2af0
- Merge branch 'cdk-1.2.x' b66f8c7182
- Fixed matchers to allow XML without new lines (closes #2832835) f9a0552430

chem-bla-ics

- Added unit tests for detection of PubChem XML files. 571f434a94
- Fixed matchers to allow XML without new lines (closes #2832835) a1f25d8629
- Added unit tests for detection of PubChem XML files. 1cec794dec
- Merge branch 'stereo' ffe9576b02
- Added reading of E/Z stereochemistry from double bonds in MDL V2000 molfiles. cb824f1896
- A minor fix to clean up a PDMD warning 024499e7c2
- Overwrite unit tests, because there are no change events passed around at all for the NoNotification interface implementations 36f295bf8a
- Added missing unit tests for IChemModel event propagation for the ICrystal field 2993e0c5a0
- Fixed propagation of change events to IChemModel when modifications are made in child IChemObjects 0c8a88fec8
- Fixed unit tests: the IChemModel.setFoo(null) should actually give a change event on the listener of the IChemModel, and not after unregistering of the Foo object. b8331764c2
- Synchronized with the Blue Obelisk version a91062b454
- Added unit test to the function of the new IO setting to force 2D coordinate output. 4e2b2bf31e
- Added writer IO option to force writing of 2D coordinates if 3D coordinates are present too, which now are preferably outputted. 0e6aa2cf14
- Added unit test to verify that if 2D and 3D coordinates are available, the 3D coordinates are outputted. 56852f8bd5
- Changed IBond.get/setStereo() to use a IBond.Stereo enumeration instead of an int (fixes #2855850): 46893ed070
- Merge branch 'cdk-1.2.x' f0c16b0c76
- Fixed Taglets: only return HTML if the Tag is really given; the toString() method is given for all cases, not just when the tag is found 1107fb2fba
- Added the Mannhold LogP descriptor 1e6b6cdfb4
- Added the Mannhold LogP descriptor to the ontology a7adc9fe5c
- Fixeda bug which was causing various parts of the DescriptorEngine to fail - it was trying to instantiate a non-descriptor class which happens to reside in the descriptor package directory. This fix is a bit kludgy - ideally only descriptors should be in that directory 0242d9ad67
- Fixes ClassCastException when not IMolecule 6f3e848f9d
- Upgraded to PMD 2.4.5 with many bug fixes, giving more accurate error reports f29a66b63a
- Added missing dependency on cdk-diff, being used in one of the unit tests 0e287dd450
- Fixed methods names to match those in the test class 789a314a8e
- Fixed test method name to match the expected patters, fixing a coverage test fail ac136190d0
- Removed duplicate code: MolecularFormulaTest now extends AbstractMolecularFormulaTest b8651c75c8
- Fixed test method annotation to point to the right method bb7d341577
- Added missing @TestMethod annotation f6f759b227

chem-bla-ics

- Added modules that were missing from the PMD testing 073e5ec96b
- Added modules that were missing from the doccheck testing 10dc19c09b
- Added reference to IUPAC documentation about stereochemistry visualization. 56adf239b0
- Merge branch 'cdk-1.2.x' 03e8496d5c
- Patch for bug 2843445. Aims to fix generation of NaN coordinates by SDG d1397fe99d
- Added missing dependency introduced by the use of AbstractFingerprinterTest in test-standard. b26eb933e6
- Updated the unit test classes for all IFingerprinter implementations to use the new AbstractFingerprinter class; a few unit tests actually fail 1989fa5c7b
- Extracted an AbstractFingerprinterTest with unit tests that should really apply to all IFingerprinter implementations 8bc42dcfc4
- Clean up of layout. 5f7cb532ee
- Fix the unit test to not give a 'input must support mark' exception on some platforms, by wrapping the InputStream in a BufferedInputStream. 6f6f41ede3
- Added missing dependencies 8759481c19
- Added ioformats to modules to test 56289e2dbc
- Use StringBuilder to aggregate the field data, which gives an huge performance boost for SD file where multiline field data is found. df35f02d32
- Use StringBuilder to aggregate the field data, which gives an huge performance boost for SD file where very much field data, like the ChEBI_complete.sdf eac8266fe9
- Factored out steps in reading the SD file data block 678e7ca206
- Bumped version, to make it clear this is not the 1.2.3 release 8c8166a1a2
- Bumped version, to make it clear this is not the 1.3.0 release eeda652998
- Fixed registering on the cdk.threadnonsage tag (closes #2796362) d451576275
- Removed obsolete pattern from old svnrev tag c8f5a727a3
- Fixed JavaDoc to remove traces of the old svnrev Tag 1a70488b81
- Synchronized exception message with implementation (fixes #2844333) c70b79cbec
- Made class private again, per authors request fa7ba022ee
- Any class will do, not just public, final and abstract dc9e8c5f59
- Two further compile fixes after the merge with CDK 1.2.x 3458dee67e
- Made the class public, to fix a compile problem introduced by the merge with CDK 1.2.x d8170d2f0e
- Added ant task to calculate JavaNCSS code statistics a8b313eace
- Added JavaNCSS 32.53 (LGPL 3.0) 6753a8ceea
- Merged from cdk-1.2.x. Also fixed some conflicts. Not sure why/who changed PharmacophoreMatcherTest to use QueryAtomContainer rather than PharmacophoreQuery 0d5689f97a
- The Pauling Electronegativity is copied in configure as well. I can't see why not copy everything we have. 3fd2b171e8
- Revert "added a test for bug 2831420": 2c2add68bb
- Patch for bug 2843445. Aims to fix generation of NaN coordinates by SDG 963b0a7980
- added a test for bug 2831420 5d1522264b
- added a test for bug #2831420 93536f0d99

chem-bla-ics

- Made InChIGeneratorFactory a singleton. 242da910d0
- Layout. af4fac7a95
- Added bug annotation 38d0235bba
- test case for bug #2846213 f84c53b98a
- Fixed perception of N.planar3 where N.sp2 was detected, by now taking into account the given hydrogen count. 1714de2663
- Fixed perception of benzene with all single bond, but hydrogen count 1 and bonds flagged aromatic. In this case, the type is C.sp2 not C.sp3. 05e0be39a0
- Added assertions to unit test for values being not null 863b0a5325
- Added two unit tests for the same problem: carbon atom types are not correctly perceived if bond order info is SINGLE only, and hydrogen count and aromaticity flag is set. f19a451a72
- Moved class into a org.openscience.cdk package, which seems to work now. I'm puzzled why it did not before. Solved several unit test fails. b055c6b0b0
- Merge branch 'cdk-1.2.x' of ssh://egonw@cdk.git.sourceforge.net/gitroot/cdk into cdk-1.2.x f77db9c186
- Unsealed the XOM jar to allow having the CustomSerializer 3b8234020c
- Fixed Javadocs error e0304bf4bd
- Fixed a wrong javadoc tag. Also removed svn tag in the SMARTS parser JJT file, replaced with git tag c8887734af
- Added support for 'public enum's 4bf822d57b
- corrected bug in bondtools.isStereo(IAtomContainer container, IAtom stereoAtom). A comparision of atom symbols in a nested loop was using the counter of the outer loop twice. Note it worked before, because there is a sort of fallback to Morgan numbers. fallback to morgan (fixes #2830287) 025fb472b8
- added a new test for bondtools 13f72bd406
- Fixed inconsistency between accepts() and write: also support writing of IAtomContainerSet and IAtomContainer as accepts() indicates (fixes #2827745) 6380578865
- General test for testing consistency between write() and accepts(), testing that all accepted IChemObject's can also be written f0678eb65a
- Added unit test for bug #2826961: inconsistent atom typing for two SMILES. Unit test does not show a fail, ruling out a CDK bug 42e45efcd9
- Remove erroneous throws statement f8cfea8bc3
- Bug found calculating the exact mass given a molecular formula when it is negative charged. 3d1de45add
- Fixed reading of the cdk/dict/data/elements.owl database which is now in OWL 73225a083a
- Fixed issue 2458210: use assertNotNull(foo) etc instead of assertTrue(foo != null). 182afe6670
- Added minimum equivalents for BondManipulator.getMaximumBondOrder() methods 6e126962ea
- Fixes asserts: after removal *no* change should be recorded 3b9fa30041
- Added IO option to disable generator of XML declaration statements in the output CML. 74451b8f0e

chem-bla-ics

- Added generics, and consistified code by always returning a List<?> of the same '?'. (And some 80 chars fixes in the JavaDocs.) d6337cd596
- Added unit tests to test that when a [Molecule|Reaction|Ring]Set has been removed from a ChemModel, the ChemModel should unregister as listener. 63e6c014a1
- Added unit tests for event propagation from [Molecule|Reaction|Ring]Sets to ChemModel. e01103543b
- More testing of flags. abb53842bf
- Fix for junior job id: [1837692] Test methods should throw only one Exception. 8c3853638e
- Fixed missing imports and wrapped to 80 chars fd2d2df6ef
- Better excpetion handling in builder3d: bc5837d848