chem-bla-ics

CDK 1.3.5

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A lot of changes in this release: the SMSD code (see doi:10.1186/1758-2946-1-12), removed outdated code (force field, R-CDK bridge), SMILES @ and @@ chiralities reading, a new IChemObjectBuilder interfaces, and several new features in the MDL IO classes. The full list:

Fix for getBestAlignmentForLabelXY eb7529b4aa

Test for getBestAlignmentForLabelXY 2cb5f4d5a9

Renamed the ligancy classes to use the term tetrahedral since they implicitly encode for tetrahedral chirality d80628ef4c

fixed PMD errors on Use instanceof against interfaces not implementations and few more Signed-off-by: Syed Asad Rahman <s9asad@gmail.com> e36a2a122e

Renamed the ligancy classes to use the term tetrahedral since they implicitly encode for tetrahedral chirality 3043c177b6

Merge branch 'cdk-1.2.x' b8110ae58d

Introducing PMD test for CDK specific issues: 406930b292

Removed unstable forcefield code 235b04fd3c

Added copyright and license header d6b6c65f5a

The createSMILES() methods now take IAtomContainer rather than IMolecule. Originally, IMolecule was the type since it was assumed that SMILES would only be generated for connected components - but the code already handles disconnected components. Since IAtomContainers are meant to support that, this change makes sense. Also a result is that we don't have to convert a IAtomContainer to IMolecule to generate SMILES 2399a18ba3

updated test cases Signed-off-by: Syed Asad Rahman <s9asad@gmail.com> 32cb936040

add on patches 4bdce612cd

fixed makeAtomsMapOfBondsMap with test 5bd8d64f62

Emergency fix: IAminoAcid instead of AminoAcid 5193626538

Merge branch 'cdk-1.2.x' 2f56fd6ddb

A few more interfaces instead of implementations 648a2f48b8

Replaced use of implementations by interfaces 6317be25ed

Use an interface instead of an implementation as type b82a2f69be

Use interfaces instead of implementation 50b9e74182

MDL reading and writing atom value line, including test cases c88bd3c0d4

chem-bla-ics

Added another test to check that a query larger than the target does not match 088afcedde

Test cases for MCS updated 15fa35a769

updated MCS solution count in the VF lib, depricated turbo MCS and provided methods for timeout c4d3bf9cad

updated test for single atom ed04f25218

Replaced outdated URL with entry in WikiPedia (fixes #3002741) ad2bd3ed63

Fixed outdated JavaDoc I forgot to remove (fixes #3002409) 82f40a1efd

Included the qm module in the dist-all (fixes #3002622) e2c95ec1dc

Cleaned up unthrown exceptions 2501371362

Removed use of SMARTS parser in the test code so that a new dependency is not required e561364152

removed unwated checks 41561a25f4

commented unused code f39566c797

test cases for the IQueryAtomContainer support in the SMSD with exceptions fixed 839827b873

test cases for the IQueryAtomContainer support in the SMSD b292f7c795

IQuery* support for the SMSD, will help in SMART based searches 75d86dd0fc

Merge branch 'master' of git@github.com:cdk/cdk 6d1a730700

Turbomode MCS search added f3f809ed50

Turbo mode MCS search added Signed-off-by: Syed Asad Rahman <s9asad@gmail.com> 8ac67bf99e

removed unwanted test case Signed-off-by: Syed Asad Rahman <s9asad@gmail.com> ea4960cda6

VF Sub search turbo mode 5b4f00a63b

Updated the SMSD code for turbo mode substructure search Refactored the SMSD class itself f5ccf1bdc8

Added two test cases by Daniel from my blog: http://chem-bla-ics.blogspot.com/2010/05/cip-rules-2-parsing-and-from-smiles.html 9cbc242454

Added two more unit tests, related to ring closing 0f4649c0d0

SMILES @ and @@ chiralities are now fully read. 2dd575ed56

chem-bla-ics

Added unit tests with various chiral SMILES situations. 4c2e9b7a96

Implemented stereo chemistry for atoms with four ligands 9abead553d

Patch to generalize the stereo chemistry handling. be1b70ac15

Merge branch 'master' of git://github.com/egonw/cdk 1d5a29bfd8

Minor fix to build.xml to ensure that SMSD code gets included in the large jar file ee5e0a21c3

Added JavaDoc testing to the QA task; removed module-uptodate which checked if the module was already compiled causing the target to be skipped a1e1f1b78f

I made sure the MDLV2000Reader considers 0,0,0 coordinates in files with a single atom as 2d and 3d coordinates. The MDLReader does not handle the 0,0,0 case explicitly, so I just added a test for 2d. It might be better to have uniforma handling, but I will file a bug report for that. 42b64e1341

The RXNReaders/Writers now all handle Atom-Atom-Mappings. This was only done in the MDLRXNReader till now 6ff55baf51

Atom-Atom-Mapping is now read and written in MDL files. Note the reading until now was into ID field, which is not in line with description of ID field in ChemObject (Returns the identifier (ID) of this object). Also added tests for MDLWriter/Reader/2000Reader. 6b787c2fd6

Flexibility for ring start angles. d6d6ab0022

more mdl reader writer tests 353f938852

Revert "Additional constant" 3b974e6238

Added a test case for short line mol files. Patch by S.Kuhn, reworked by M.Rijnbeek. c4ea1d843f

MDL reading and writing UP_OR_DOWN e36983b165

Merge branch 'master' of git@github.com:cdk/cdk d694d197fb

Removal of references to removed R-CDK bridge fd1e57c615

Removed the R-based model package and associated jar files and test code 5733da3fdd

Merge branch 'master' of git@github.com:egonw/cdk 0d3a0c9f1e

Removal of references to removed R-CDK bridge b1075d7df0

Removed the R-based model package and associated jar files and test code e41372becb

Removal of references to removed R-CDK bridge d3f65d0615

Removed DocCheck from Eclipse' Build Path fcd762373c

chem-bla-ics

Removed obsolete castings, or replaced by more general ones b34423dfcd

added @Test Signed-off-by: Syed Asad Rahman <s9asad@gmail.com> eebdb3d001

added CDKRMapHandlerTest 82b9faf52e

added CDKRMapHandlerTest Signed-off-by: Syed Asad Rahman <s9asad@gmail.com> bb7bcb46fa

The big SMSD patch. 10edb71d6e

Merge branch 'cdk-1.2.x' f17fc8fb40

Fixed a ClassCastException in a unit test; I messed up (mea culpa) b5fa3dca01

Copied code from the DefaultChemObjectBuilder to handle the IBond constructor that takes an IAtom[] which I had forgotten to port to DebugChemObjectBuilder and NoNotificationChemObjectBuilder (fixes a few regressions) 25427b41ea

Merge branch 'cdk-1.2.x' 426558e934

Fixed NullPointerExceptions for LonePair's and SingleElectron's constructed with the no-argument constructors 5f34897eb8

Added missing cloning of single electrons 2d4c1220c3

Do not try to clone the atom if it does not exist 9672df0df7

MDL reading and writing valency c20a0ea691

Line separator fix for RGroup writer ad706cc834

de-Javadoc numerous comments (fixes #2980066) 4fc483724a

More extensive testing for removeHydrogens in atomcontainers with hetero atoms without Hs 3155d7dc56

Merge branch 'cdk-1.2.x' bc8972ce6d

Be a bit more forthcoming with debug messages: report also the parameter types of the method 0f85f52dda

Merge branch 'master' of git@github.com:egonw/cdk c98a7aff57

This patch makes sure that the removeHydrogens method in AtomContainerManipulator sets hydrogenCoutn to 0 if no hydrogens were on a heavy atom. Till now, this was null, which was at least not good, in a way even wrong. 708cf8ac03

converted uses of indexOf to startsWith/contains 7b9d84e44a

Updated HIN reader to fix bug 2984581 f95c6324a8

chem-bla-ics

Added unit test to see of arrays are properly cloned, and that array entries of the original are not overwritten 38d5f8d191

Unit test that the IAtom[] array is properly cloned, and overwriting entries in the clone does not overwrite entries on the original 3c1b07e26f

Removed duplication of cloning. 216c1600b9

Apparently the super.clone() does not clone the pointer to the IAtomContainer[], causing a clone() followed by changing containers in the clone to overwrite the original IAtomContainer[]. Fixed by creating a new array. 4e5d6a120f

Moved test from the specific class to the abstract tests, as the behavior should be the same for NNMoleculeSet and DebugMoleculeSet too 068fb3b9b2

Fixed a typo in the test method name 8142ae5fa1

Got rid of some debug prints 6079160811

Fixed a regex bug which prevented the engine from properly loading descriptor class names 9bd0490de5

Some code cleanup to make it more idiomatic Java 565d7c369e

New IChemObjectBuilder interface: 45f683f1ff

Two more tests for the issue: atom typing works fine; aromaticity detection fails: one ring is detected as aromatic (that with two nitrogesn), so that it does not consider the double ring, marking the other ring as non-aromatic 3be2367b36