

Profiling the CDK atom typer

Egon Willighagen 

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Keywords

Cdk, Java

Abstract

I was doing some profiling (YourKit and Eclipse3.4) of the CDK atom typer, and it turns out that most time is spent on the perception of nitrogen atom types, which seems to be caused by the `loadClassInternal()` method of the JVM (java-1.5.0-sun-1.5.0.16 on Ubuntu Hardy):

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chem-bla-ics

I was doing some profiling ([YourKit](#) and Eclipse3.4) of the CDK atom typer, and it turns out that most time is spent on the perception of nitrogen atom types, which seems to be caused by the `loadClassInternal()` method of the JVM (java-1.5.0-sun-1.5.0.16 on Ubuntu Hardy):

+	org.openscience.cdk.atomtype.CDKAtomTypeMatcher.findMatchingAtomType(IAtomContainer, IAtom)	3,634	100%
-	org.openscience.cdk.atomtype.CDKAtomTypeMatcher.perceiveNitrogens(IAtomContainer, IAtom)	2,793	77%
-	org.openscience.cdk.atomtype.CDKAtomTypeMatcher.isRingAtom(IAtom, IAtomContainer)	1,670	46%
+	org.openscience.cdk.graph.SpanningTree.getConnectedComponents()	846	23%
+	org.openscience.cdk.graph.SpanningTree.<init>(IAtomContainer)	412	11%
+	java.lang.ClassLoader.loadClassInternal(String)	410	11%
-	org.openscience.cdk.atomtype.CDKAtomTypeMatcher.getRing(IAtom, IAtomContainer)	1,031	28%
-	org.openscience.cdk.graph.SpanningTree.getAllRings()	897	25%
-	org.openscience.cdk.graph.SpanningTree.getBasicRings()	893	25%
-	org.openscience.cdk.DefaultChemObjectBuilder.newRingSet()	801	22%
-	java.lang.ClassLoader.loadClassInternal(String)	800	22%
+	org.openscience.cdk.graph.SpanningTree.getRing(IAtomContainer, IBond)	83	2%
+	org.openscience.cdk.graph.SpanningTree.getSpanningTree()	6	0%
+	org.openscience.cdk.AtomContainerSet.addAtomContainer(IAtomContainer)	1	0%
+	org.openscience.cdk.graph.SpanningTree.combineRings(IRingSet, int, int)	2	0%
+	org.openscience.cdk.graph.SpanningTree.getConnectedComponents()	103	3%
+	org.openscience.cdk.graph.SpanningTree.<init>(IAtomContainer)	30	1%
+	org.openscience.cdk.atomtype.CDKAtomTypeMatcher.getAtomType(String)	46	1%
+	org.openscience.cdk.atomtype.CDKAtomTypeMatcher.isAcceptable(IAtom, IAtomContainer, IAto	9	0%
+	org.openscience.cdk.atomtype.CDKAtomTypeMatcher.isAmide(IAtom, IAtomContainer)	7	0%
+	org.openscience.cdk.atomtype.CDKAtomTypeMatcher.isThioAmide(IAtom, IAtomContainer)	6	0%
+	org.openscience.cdk.atomtype.CDKAtomTypeMatcher.bothNeighborsAreSp2(IAtom, IAtomCont	5	0%
+	org.openscience.cdk.AtomContainer.getConnectedBondsCount(IAtom)	3	0%
+	org.openscience.cdk.atomtype.CDKAtomTypeMatcher.perceiveNitrogenRadicals(IAtomContain	2	0%
-	org.openscience.cdk.AtomContainer.getMaximumBondOrder(IAtom)	2	0%
-	org.openscience.cdk.atomtype.CDKAtomTypeMatcher.hasOneSingleElectron(IAtomContainer, I	1	0%
-	org.openscience.cdk.AtomContainer.getConnectedAtomsCount(IAtom)	1	0%
+	org.openscience.cdk.atomtype.CDKAtomTypeMatcher.perceiveCarbons(IAtomContainer, IAtom)	482	13%
+	org.openscience.cdk.atomtype.CDKAtomTypeMatcher.perceiveHalogens(IAtomContainer, IAtom)	73	2%