

# Profiling the CDK atom typer

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## Keywords

Cdk, Java

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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 spend 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.getCyclicFragmentsContainer()	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.getCyclicFragmentsContainer()	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, IAtom)	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, IAtomContainer)	5	0%
org.openscience.cdk.AtomContainer.getConnectedBondsCount(IAtom)	3	0%
org.openscience.cdk.atomtype.CDKAtomTypeMatcher.perceiveNitrogenRadicals(IAtomContainer)	2	0%
org.openscience.cdk.AtomContainer.getMaximumBondOrder(IAtom)	2	0%
org.openscience.cdk.atomtype.CDKAtomTypeMatcher.hasOneSingleElectron(IAtomContainer, IAtom)	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%