

Bioclipse for CDK Developers #2

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Keywords

Cdk, Bioclipse

Abstract

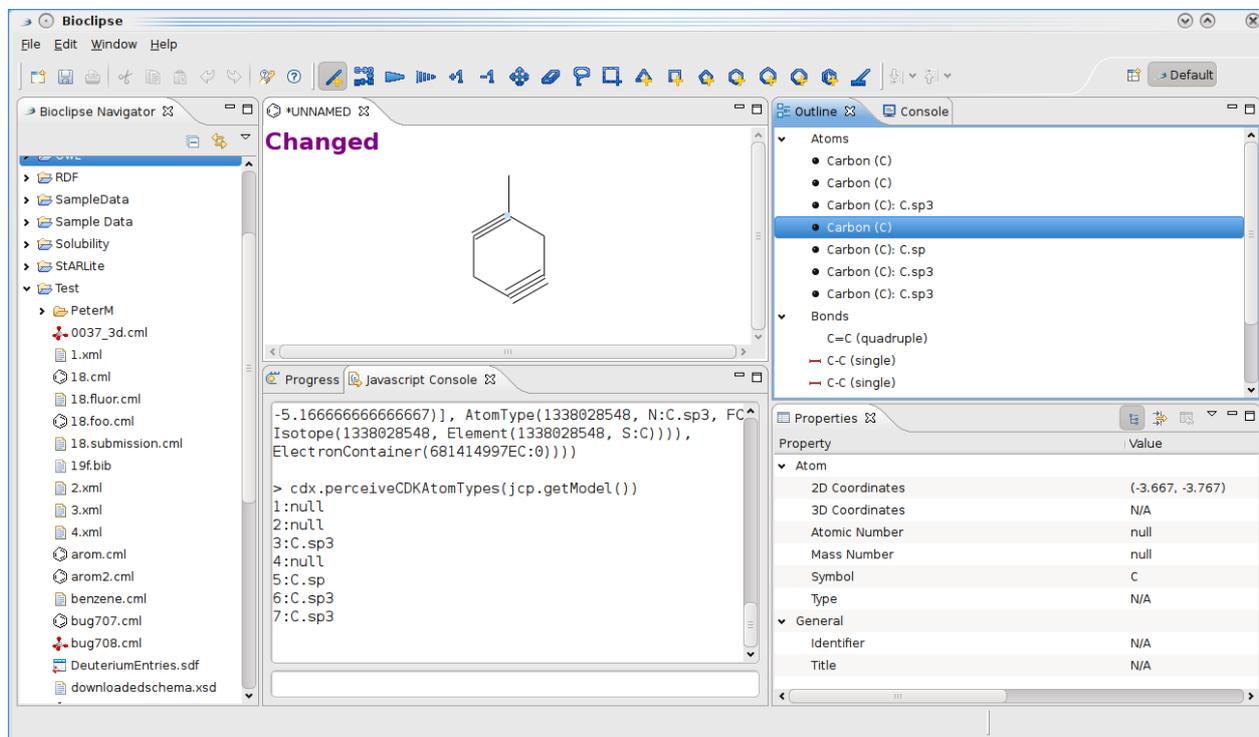
I reported earlier how Bioclipse allows you to use a script to perceive atom types for the content of the JChemPaint RCP editor. This functionality is now available in the outline, and indicates directly if Bioclipse (and the underlying CDK) understands the chemistry you are drawing. In a future Bioclipse release, these problems will be visualized more prominently, likely using the Errors/Problems Views available from Eclipse, or otherwise.

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chem-bla-ics

I [reported earlier](#) how [Bioclipse](#) allows you to use a script to perceive atom types for the content of the JChemPaint RCP editor. This functionality is now available in the outline, and indicates directly if Bioclipse (and the underlying [CDK](#)) understands the chemistry you are drawing. In a future Bioclipse release, these *problems* will be visualized more prominently, likely using the Errors/Problems Views available from Eclipse, or otherwise.



The screenshot displays the Bioclipse IDE interface. The central workspace shows a chemical structure of a substituted benzene ring with a methyl group and a double bond. The word "Changed" is written in purple above the structure. The left sidebar contains a project tree with folders like "Test" and "PeterM", and files such as "0037_3d.cml", "1.xml", "18.cml", "18.fluor.cml", "18.foo.cml", "18.submission.cml", "19f.bib", "2.xml", "3.xml", "4.xml", "arom.cml", "arom2.cml", "benzene.cml", "bug707.cml", "bug708.cml", "DeuteriumEntries.sdf", and "downloadedschema.xsd". The bottom console shows a JavaScript script and its output:

```
> cdx.perceiveCDKAtomTypes(jcp.getModel())
1:null
2:null
3:C.sp3
4:null
5:C.sp
6:C.sp3
7:C.sp3
```

The right sidebar contains an "Outline" view listing atoms and bonds:

- Atoms
 - Carbon (C)
 - Carbon (C)
 - Carbon (C): C.sp3
 - Carbon (C)
 - Carbon (C): C.sp
 - Carbon (C): C.sp3
 - Carbon (C): C.sp3
- Bonds
 - C=C (quadruple)
 - C-C (single)
 - C-C (single)

The bottom right pane shows the "Properties" view for the selected atom:

Property	Value
Atom	
2D Coordinates	(-3.667, -3.767)
3D Coordinates	N/A
Atomic Number	null
Mass Number	null
Symbol	C
Type	N/A
General	
Identifier	N/A
Title	N/A