

chem-bla-ics

# Bioclipse for CDK Developers #2

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## Keywords

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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 main window shows a chemical structure editor with a benzene ring and a methyl group. The word "Changed" is written in purple above the structure. The left sidebar contains a Bioclipse Navigator with a tree view of files and folders, including "Test" and "PeterM". The bottom-left pane shows a JavaScript console with the following output:

```
-5.166666666666667]], AtomType(1338028548, N:C.sp3, FC^  
Isotope(1338028548, Element(1338028548, S:C))),  
ElectronContainer(681414997EC:0)))  
> 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 showing a tree of 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 a 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