

Bioclipse2 Scripting #1: from SMILES to a UFF optimized structure in Jmol

Egon Willighagen 

Published October 25, 2008

Citation

Willighagen, E. (2008). Bioclipse2 Scripting #1: from SMILES to a UFF optimized structure in Jmol. In *chem-bla-ics*. chem-bla-ics. <https://doi.org/10.59350/5azgt-k8a94>

Keywords

Bioclipse, Cml, Cdk, Jmol, Eclipse

Abstract

After some difficulties this week with making an export of CDK plugins in the Bioclipse2 Cheminformatics feature of with the cdk-eclipse software, I got the following cute Bioclipse2 script up and running:

Copyright

Copyright © Egon Willighagen 2008. Distributed under the terms of the [Creative Commons Attribution 4.0 International License](https://creativecommons.org/licenses/by/4.0/), which permits unrestricted use, distribution, and reproduction in any medium, provided the original author and source are credited.

chem-bla-ics

After some difficulties this week with making an export of [CDK](#) plugins in the [Bioclipse2](#) *Cheminformatics* feature of with the [cdk-eclipse](#) software, I got the following cute Bioclipse2 script up and running:

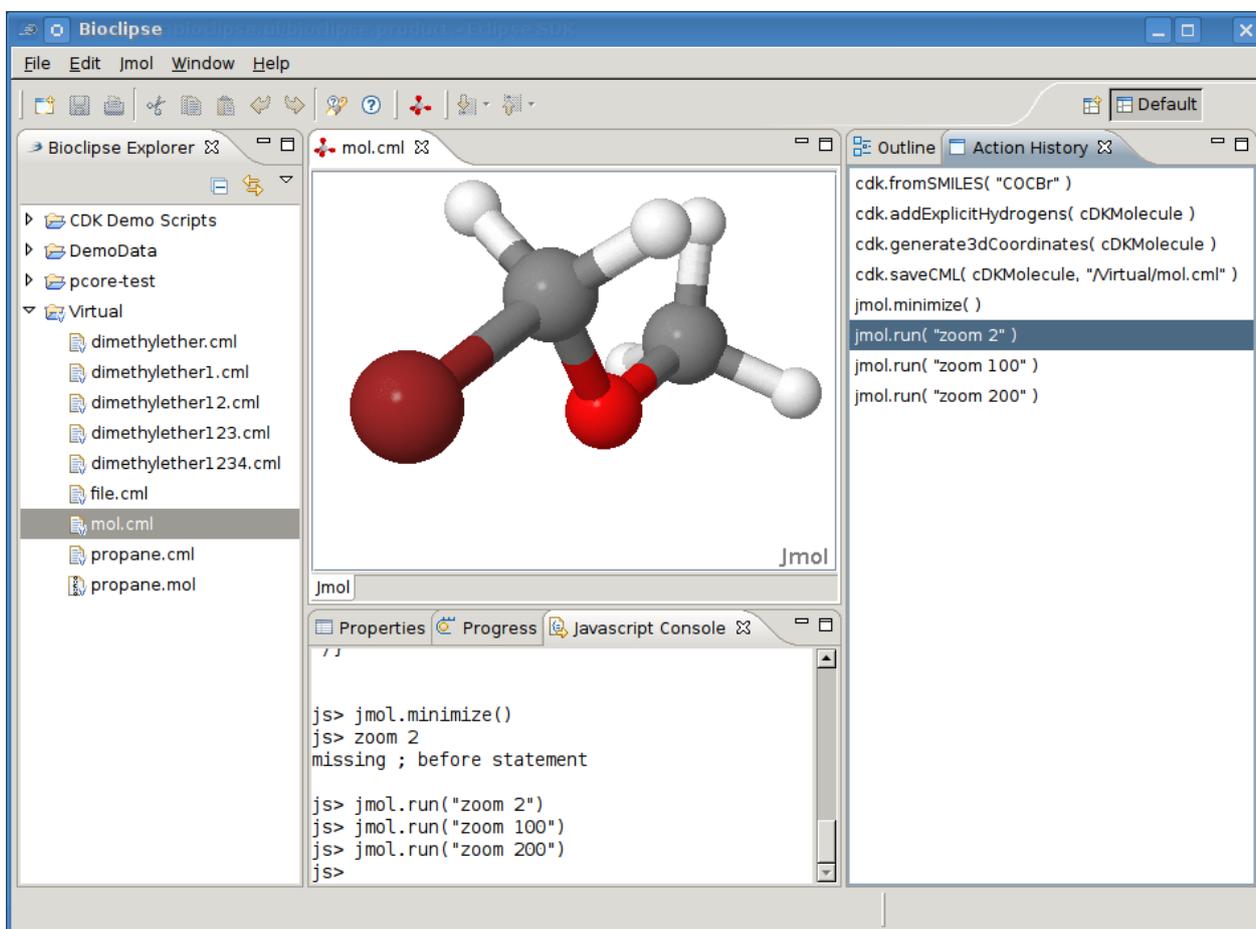
```
dimethylether = cdk.fromSMILES( "COC" );
cdk.addExplicitHydrogens( dimethylether );
cdk.generate3dCoordinates( dimethylether );

// save as CML
cdk.saveCML( dimethylether, "/Virtual/dimethylether.cml" );
ui.open( "/Virtual/dimethylether.cml" ); // this should open a JmolEditor

jmol.minimize();
```

You can see four of my favorite cheminformatics tools integrated: CDK is used to convert a SMILES into connection table with add explicit hydrogens, and to create initial 3D coordinates (with the code from Christian Hoppe, and thanx to Stefan for fixing that code in the CDK 1.1.x branch!). Then, [CMLDOM](#) is used to create and save a CML document, which is then opened into a [Jmol](#) editor in Bioclipse.

A variation of this script is visible in the following screenshot:



chem-bla-ics

This and other Bioclipse2 scripts I will post in [Gist](#), a sort of [pastebin](#) supporting version history, and I'll tag them with *bioclipse gist* on [delicious](#), so that you can always browse them, comment on them, or add your own gists at <http://delicious.com/tag/bioclipse+gist>.