

chem-bla-ics

JChemPaint for Bioclipse2

Egon Willighagen 

Published April 28, 2008

Citation

Willighagen, E. (2008). JChemPaint for Bioclipse2. In *chem-bla-ics*. chem-bla-ics. <https://doi.org/10.59350/gqaxm-b3d59>

Keywords

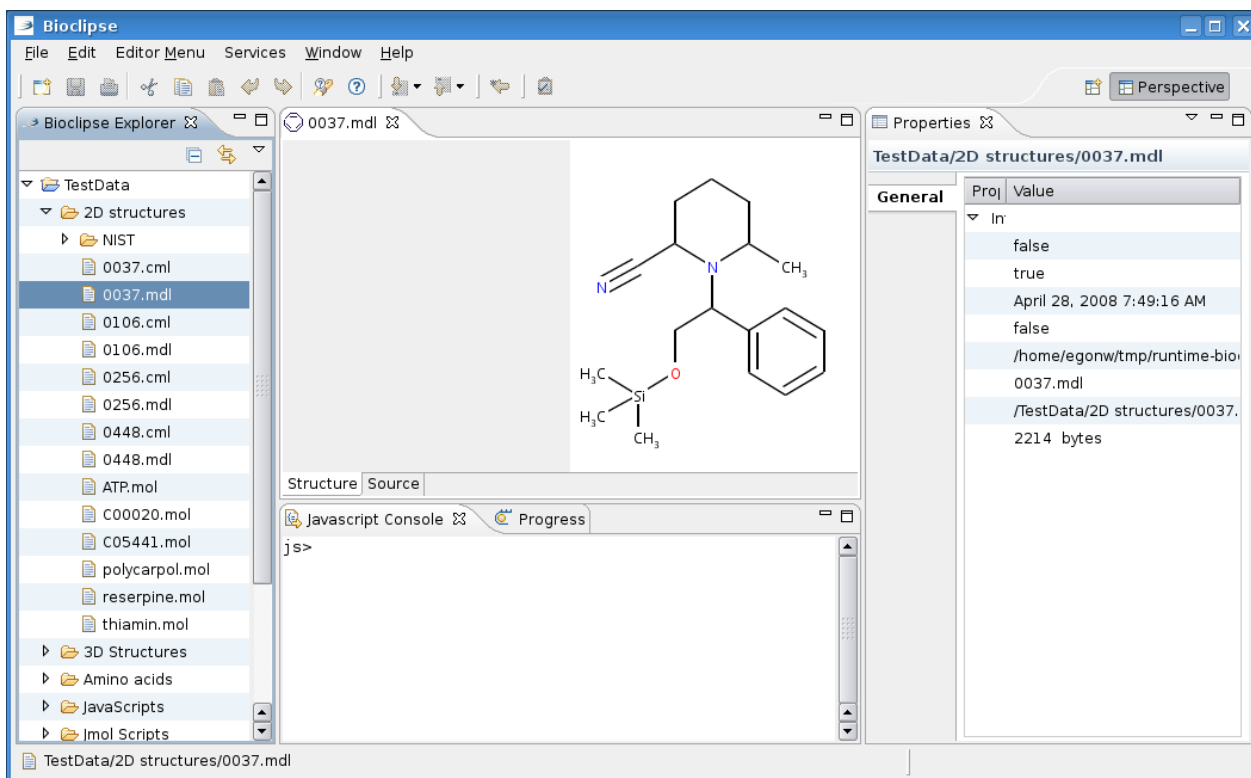
Bioclipse, Jchempaint

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

Today [Ola](#), Jonathan and I have a mini-hack session on getting [JChemPaint](#) support ported from Bioclipse1 to [Bioclipse2](#). And, we made some progress:



The screenshot displays the Bioclipse2 application window. The main editor shows a chemical structure of a complex molecule with a piperidine ring, a nitrile group, a methyl group, a benzene ring, and a trimethylsilyloxy group. The interface includes a menu bar (File, Edit, Editor Menu, Services, Window, Help), a toolbar, a Bioclipse Explorer on the left with a file tree, a Properties panel on the right showing details for 'TestData/2D structures/0037.mdl', and a Javascript Console at the bottom.

Proj	value
In:	
	false
	true
	April 28, 2008 7:49:16 AM
	false
	/home/egonw/tmp/runtime-bio...
	0037.mdl
	/TestData/2D structures/0037.
	2214 bytes

I'm sure there is still a lot to do, but this is promising... :)

Oh, and BTW, this is based on the JChemPaint 2.3 / CDK 1.0.2 branch, in case you are interested in those details.