

Small java applet for 2D structure drawing

Egon Willighagen 

Published August 18, 2006

Citation

Willighagen, E. (2006). Small java applet for 2D structure drawing. In *chem-bla-ics*. chem-bla-ics. <https://doi.org/10.59350/269sm-8sn42>

Keywords

Java

Abstract

Trepalin et al. published in *Molecules* the article A Java Chemical Structure Editor Supporting the Modular Chemical Descriptor Language (MCDL) (open access PDF). The applet is about 250kB (though the article mentions 200kB) in size and downloadable from the MCDL project on SourceForge (license: Public Domain). The article compares the applet with the JChemPaint applet and notes that their applet is much smaller.

Copyright

Copyright © Egon Willighagen 2006. 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

Trepalin et al. published in [Molecules](#) the article *A Java Chemical Structure Editor Supporting the Modular Chemical Descriptor Language (MCDL)* (open access [PDF](#)). The applet is about 250kB (though the article mentions 200kB) in size and downloadable from the [MCDL](#) project on SourceForge (license: Public Domain). The article compares the applet with the [JChemPaint](#) applet and notes that their applet is much smaller. Both allow a template database for automated structure diagram generation, and the database that comes with the MCDL applet contains 105 fragments, whereas the JChemPaint applet contains a few.

The article also discusses the algorithm they use to deduce bond orders, starting from the MCDL, a problem [CDK](#) is struggling with when dealing with SMILES strings.