Small java applet for 2D structure drawing

Citation

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.

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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.