

Janocchio: Jmol and CDK based ^1H coupling constant prediction

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Keywords

Jmol, Cdk, Nmr

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chem-bla-ics

While looking up a reference for [FirstGlance in Jmol](#), I found [Janocchio](#), a [CDK](#) and [Jmol](#) based tool for prediction of coupling constants, [recently published](#) in [Magnetic Resonance in Chemistry](#). It's written by Evans, Bodkin, Baker and Sharman (from [Eli Lilly](#)) and licensed LGPL. It is one of those rare contributions of pharmaceutical industry, and I can only deeply appreciate this contribution.

A quote from the article:

- *It was therefore decided to create a Java application and applet, 'JAvA NOe and Coupling Calculator with Handy Interactive Operation' (Janocchio), using the open source libraries of the molecular viewer Jmol and the Chemical Development Kit (CDK). It aims to provide a simple and intuitive way to calculate both the NOEs and couplings.*

Release 1.0.1 of last May uses an old Jmol, and the CDK release from 26 August 2005. A bit outdated, and I am wondering if it would be a lot of work to integrate this into Bioclipse. [Maybe a summer job?](#)