chem-bla-ics

Janocchio: Jmol and CDK based 1H coupling constant prediction

Egon Willighagen

Published June 10, 2007

Citation
Willighagen, E. (2007). Janocchio: Jmol and CDK based 1H coupling constant prediction. In *chem-bla-ics*. chem-bla-ics. https://doi.org/10.59350/rxzh8-9yr48

Keywords
Jmol, Cdk, Nmr

Abstract
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.

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 A bit outdated, and I am wondering if it would be a lot of work to integrate this into Bioclipse.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?