jcp

NAME

jcp – Open the JChemPaint structure editor

DESCRIPTION

The command *jcp* opens the *JChemPaint* structure editor, a public domain product under the LPGL license. The current WEB page is http://sourceforge.net/apps/mediawiki/cdk/index.php?title=JChemPaint.

You can view, modify, and compose chemical structures. When *jcp* is entered and a TopSpin dataset is open containing a *mol* file in its expno or procno directory, the respective structure will be loaded automatically into *JChemPaint*. Otherwise *JchemPaint* will be opened with an empty drawing area. You may browse for structures or immediately start drawing a new structure.

OUTPUT FILES

When you draw a structure with *JchemPaint,* it is recommended to store it as *mol file* in a TopSpin dataset in the expno or procno directory. Then the structure can be used by various other TopSpin functionalities such a structure elucidation, multiplet analysis, chemical shift prediction, or structure/spectra consistency analysis.