

chem-bla-ics

The SWT JChemPaint (viewing) widget

Egon Willighagen 

Published June 18, 2008

Citation

Willighagen, E. (2008). The SWT JChemPaint (viewing) widget. In *chem-bla-ics*. chem-bla-ics. <https://doi.org/10.59350/895qm-mnq80>

Keywords

Cdk, Jchempaint, Bioclipse

Copyright

Copyright © Egon Willighagen 2008. The work is made available under the [Creative Commons CC0 public domain dedication](#).

chem-bla-ics

In addition to this [Swing-based screenshot of JChemPaint](#), here's a SWT widget in action (lower right corner):

The screenshot displays the Bioclipse application window. The main area is divided into several panels:

- Structure table:** A table with columns: Ind., Structure, ROTB, LOGP, INFO, DONH, and TPS. It contains two entries:

Ind.	Structure	ROTB	LOGP	INFO	DONH	TPS
1		5	2.1420000000	CTANGIBLEWEE	1	5.7295600
2		5	2.4770000000	CTANGIBLE	1	5.7295600

- Outline:** A list of entries with numerical IDs and values in scientific notation, such as 0: [5, 9.080000000000000e-001], 1: [5, 2.142000000000000e+000], etc.
- 2D-Structure (Single M):** A 2D chemical structure viewer showing a molecule with a sulfur atom (S), a nitrogen atom (N), and a chlorine atom (Cl).
- JavaScript Console:** A console window with the prompt `js>`.

Not quite as beautiful as the [ChemWriter](#), but a start.