



CORINA Classic Interactive Demo

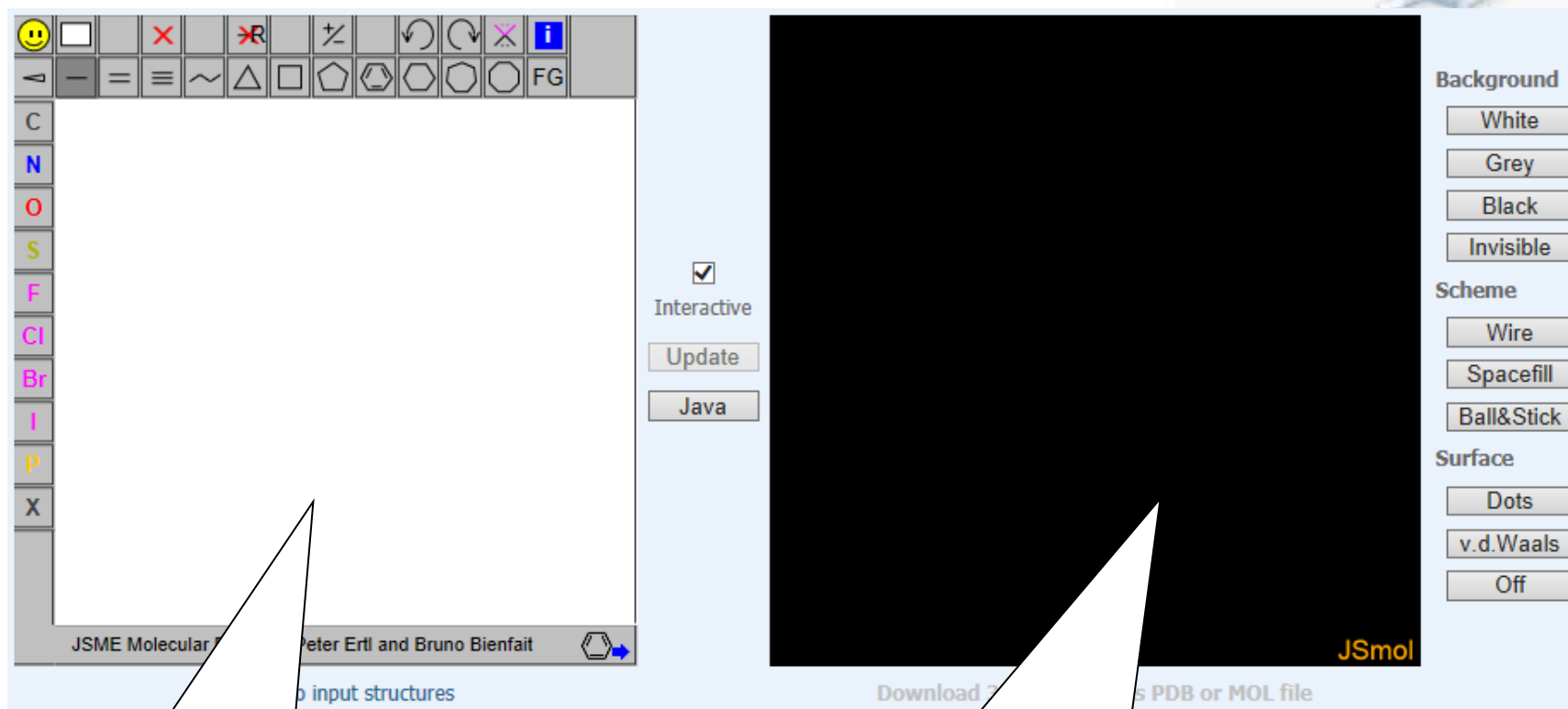
Short User Guide

Molecular Networks GmbH
Neumeyerstr. 28
90411 Nürnberg, Germany

mn-am.com

Altamira LLC
1455 Candlewood Drive
Columbus, Ohio 43235, USA

CORINA Classic Interactive



Sketch a molecule ...

... and the 3D structure will be generated and displayed simultaneously

CORINA Classic Interactive



Start drawing L-Alanine ...

... continue drawing ...

CORINA Classic Interactive



... finished sketching

Download PDB or Molfile with 3D coordinates

```

corina 05271317283D 1 1.00000 0.00000 0
CORINA 3.48 0000 08.02.2010
13 12 0 0 0 0 999 V2000
0.9220 1.1080 -0.6071 O 0 0 0 0 0 0 0 0 0 0 0 0
0.7009 0.1028 0.0258 C 0 0 0 0 0 0 0 0 0 0 0 0
-0.7113 -0.2429 0.4221 C 0 0 2 0 0 0 0 0 0 0 0 0
-0.7169 -0.6405 1.4370 H 0 0 0 0 0 0 0 0 0 0 0 0
-1.2685 -1.2936 -0.5404 C 0 0 0 0 0 0 0 0 0 0 0 0
-1.5455 0.9650 0.3648 N 0 0 0 0 0 0 0 0 0 0 0 0
1.7133 -0.7061 0.3759 O 0 0 0 0 0 0 0 0 0 0 0 0
-0.6495 -2.1898 -0.4979 H 0 0 0 0 0 0 0 0 0 0 0 0
-2.2900 -1.5436 -0.2538 H 0 0 0 0 0 0 0 0 0 0 0 0
-1.2629 -0.8959 -1.5553 H 0 0 0 0 0 0 0 0 0 0 0 0
-1.2367 1.6500 1.0383 H 0 0 0 0 0 0 0 0 0 0 0 0
-1.5566 1.3529 -0.5665 H 0 0 0 0 0 0 0 0 0 0 0 0
2.6016 -0.4427 0.0990 H 0 0 0 0 0 0 0 0 0 0 0 0
1 2 2 0 0 0 0
2 3 1 0 0 0 0
2 7 1 0 0 0 0
3 4 1 0 0 0 0
3 5 1 0 0 0 0
    
```

Copy & Paste

The screenshot shows the CORINA Classic software interface. On the left, a Notepad++ window displays a Molfile for L-Alanine. The main window shows a 2D chemical structure of L-Alanine with a context menu open, offering options: 'Copy as SMILES', 'Copy as MOL', and 'Paste MOL or SDF'. To the right, the JSmol viewer displays a 3D ball-and-stick model of the molecule with a surface representation. The JSmol control panel on the far right includes options for Background (White, Grey, Black, Invisible), Scheme (Wire, Spacefill, Ball&Stick), and Surface (Dots, v.d.Waals, Off). Buttons for 'Interactive', 'Update', and 'Java' are also visible.

```
1 L-Alanine
2
3
4 7 6 0 0 1 0 0 0 0 0 0 0999 V2000
5 9.6605 -3.5645 0.0000 C 0 0 2 0 0 0
6 10.3749 -3.1521 0.0000 C 0 0 0 0 0 0
7 10.3750 -2.3272 0.0000 O 0 0 0 0 0 0
8 11.0893 -3.5646 0.0000 O 0 0 0 0 0 0
9 8.9461 -3.1520 0.0000 N 0 0 0 0 0 0
10 9.2205 -4.2611 0.0000 N 0 0 0 0 0 0
11 10.0638 -4.2611 0.0000 H 0 0 0 0 0 0
12 1 2 1 0 0 0 0 0
13 2 3 2 0 0 0 0 0
14 2 4 1 0 0 0 0 0
15 1 5 1 0 0 0 0 0
16 1 6 1 1 0 0 0 0
17 1 7 1 6 0 0 0 0
18 M END
19
```

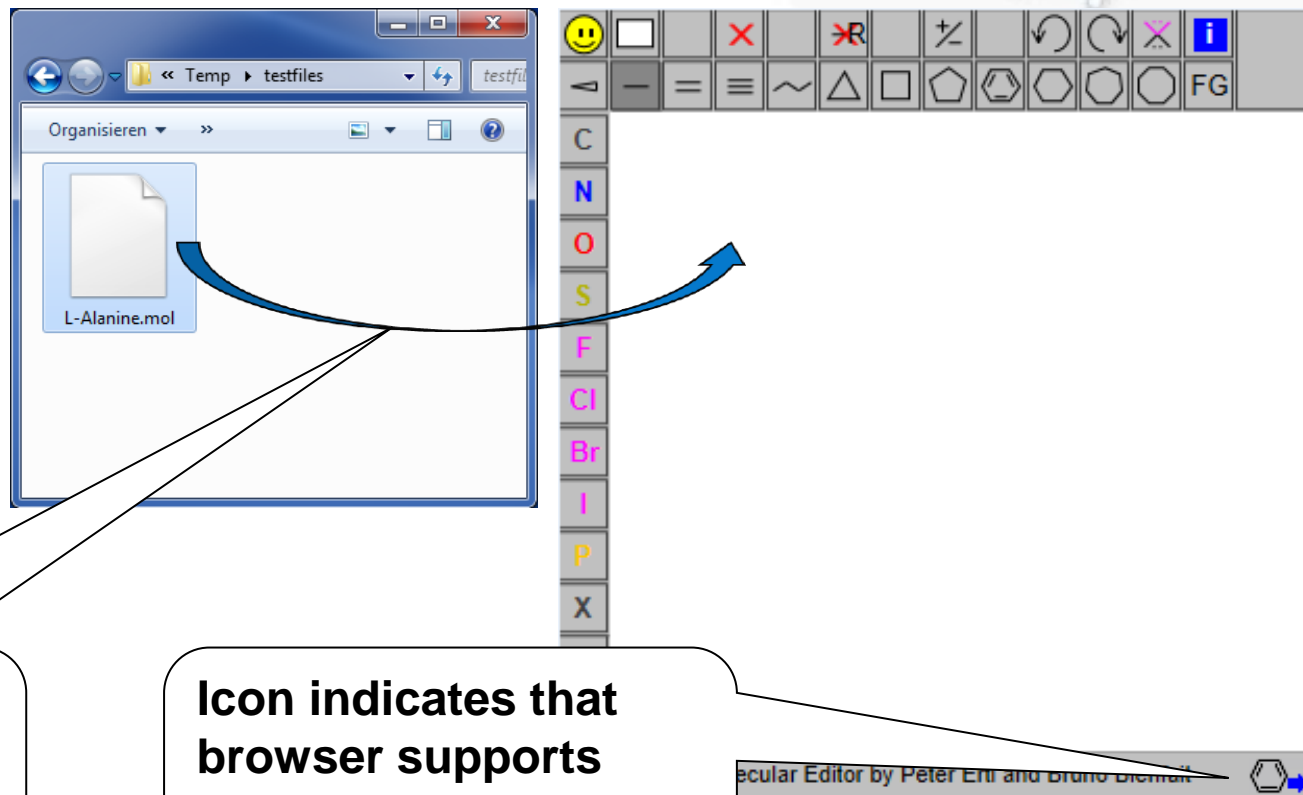
Open a Molfile in a text editor, select all (Ctrl-a), copy (Ctrl-c)

Paste structure into JSME (Ctrl-v) or use context menu (Paste MOL or SDF)

3D structure is generated and displayed on the fly

Drag & Drop

- Requires HTML5 compatible browser (IE 10, Firefox 19, Chrome 24)
- Import of MOL files











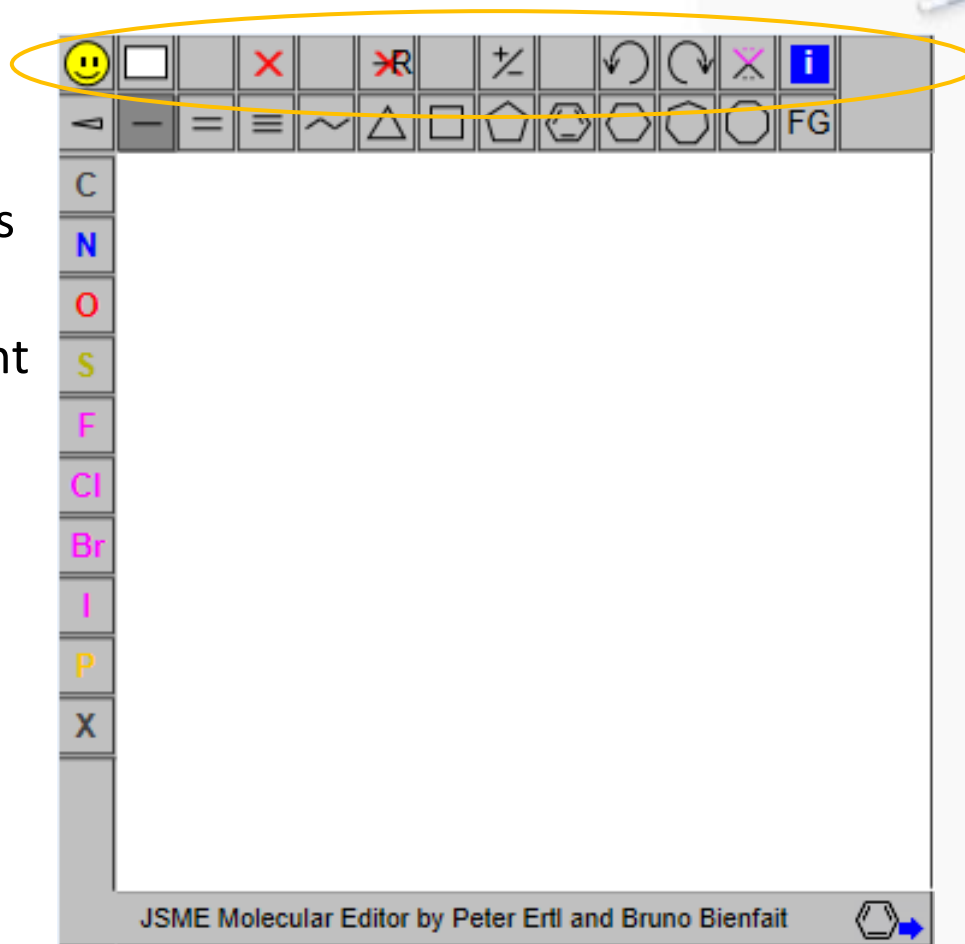
Drag and Drop MOL file from file explorer to JSME

Icon indicates that browser supports Drag and Drop functionality

Molecule Editor JSME (1/3)

■ Functionality

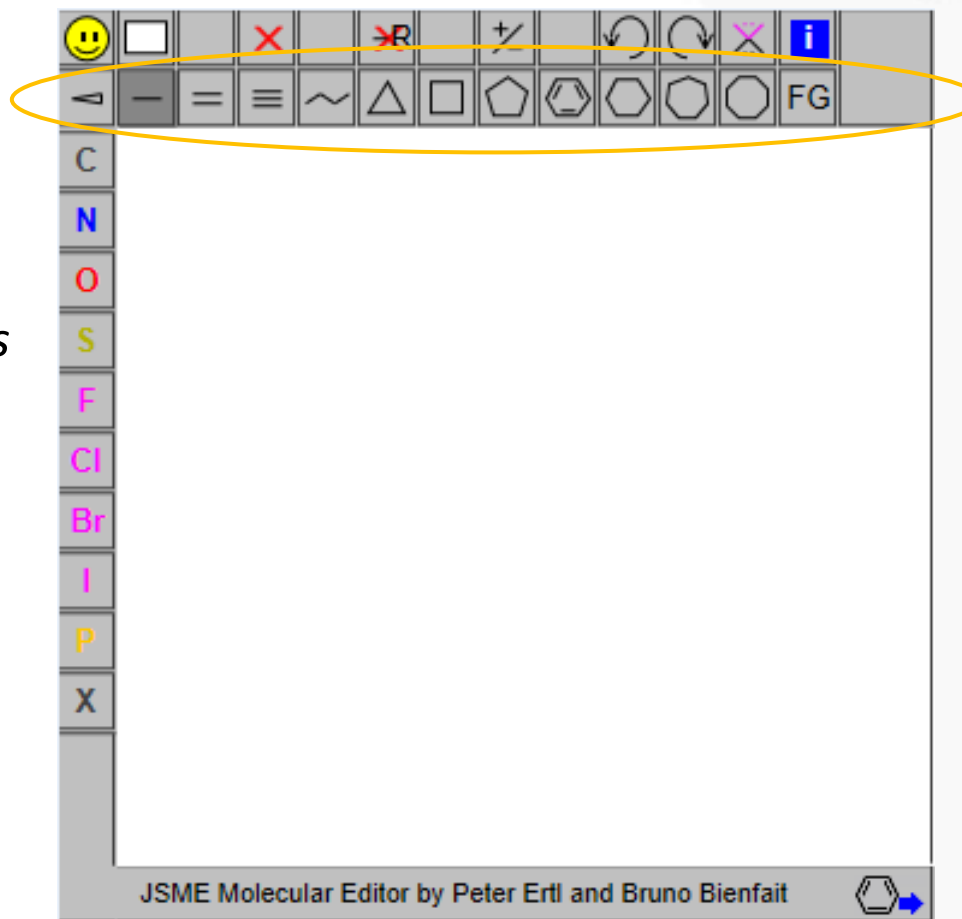
-  Clear canvas
-  Delete atoms and bonds by clicking them
-  Delete entire substituent
-  Change formal charges on atoms
-  Undo last step
-  Redo last step
-  Next ring as spiro
-  About JSME



Molecule Editor JSME (2/3)

■ Functionality

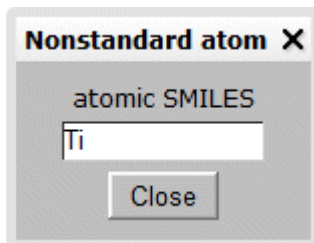
- *Select bond types*
- *Draw linear chains*
- *Select ring templates*
- *Select functional groups (FG), e.g., nitro, carboxylic acid, ester, etc.*



Molecule Editor JSME (3/3)

■ Functionality

- *Select specific atom types*
- *Press "X" to input atom type not listed*

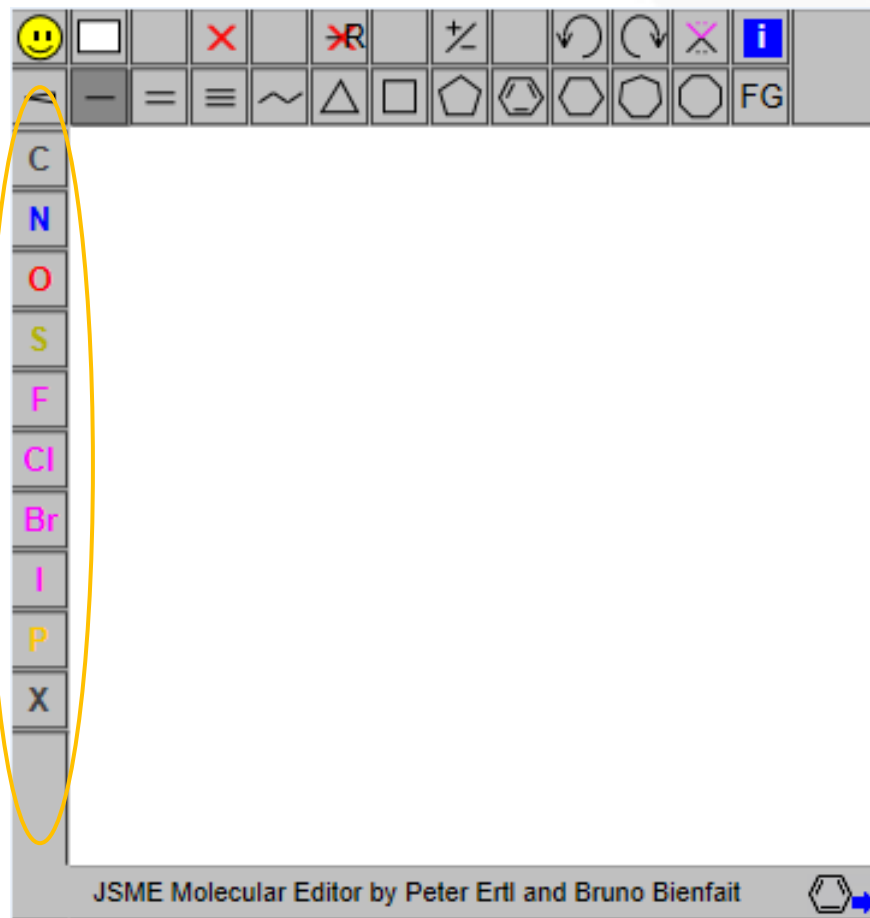


Nonstandard atom X

atomic SMILES

Close

- *Press "Close" to add atom*



The image shows the JSME Molecular Editor interface. At the top is a toolbar with various icons for drawing and editing. Below the toolbar is a vertical menu of atom types: C, N, O, S, F, Cl, Br, I, P, and X. The 'X' button is circled in yellow. The main editing area is empty. At the bottom, there is a footer that reads 'JSME Molecular Editor by Peter Ertl and Bruno Bienfait' and a small icon of a benzene ring with a blue arrow pointing to the right.



Thank you for following this user guide!
mn-am.com