

Ctrl+Z Ctrl+Y Ctrl+H X Ctrl+F = Shift-

Information

Title: New design

Keep source properties

Notes: New design DPPIV

Radial Plot

0.660 Pred (O2 Field for ...

MW Sim

ability TPSA SlogP

Actions

Add H Del H

Charge for pH7 Add Fields

Minimize

Optimize Alignment

Save a Copy

OK Align Cancel

Atom RMB+click

Undo Minimize Ctrl+Z

Redo Ctrl+Y

Select All Ctrl+A

Invert Selection Ctrl+I

Select Fragment

Paste Ctrl+V

Recenter View Home

Center on selection End

Delete Del

Set Element

Charge

Save Image As...

Hydrogen H

Carbon C

Nitrogen N

Oxygen O

Fluorine F

Phosphorus P

Sulfur S

Chlorine Cl

Bromine Br

Iodine I

Make Positive +

Make Neutral 0

Make Negative -

Hover mouse to change element: N/O/S/F

Score: 0.866 | O2 Field for Median(pIC50) [Pred 6.7; Dist to model Excellent]

LM rotate, RM translate, MM scales. Shift-LM/RM moves coordinates. Drag on an atom to draw.

Shortcut	Action	Shortcut	Action	Shortcut	Action
Shift + </>	Zoom in/out	LMB-drag on white space	Rotate all objects	LMB-click on atom + atom selected in drawing widget	Change atom type
RMB-click on white space	Display menu	Shift+ LMB-drag on white space	Rotate molecule relative to Ref/Prot	LMB-click on atom + ring selected in drawing widget	Growing a ring
RMB-click on any atom	Display long menu	RMB-drag on white space	Translate all objects	RMB-drag on atom	Move selected atom
L/RMB	Left/Right mouse button	Shift+RMB-drag on white space	Translate molecule relative to Ref/Prot		

The screenshot displays the Molecule Editor interface. The main window shows a 3D ball-and-stick model of a complex organic molecule. Several annotations with red arrows point to specific parts of the molecule:

- "LMB-drag to rotate the smaller group" and "Shift-LMB drag to rotate the bigger group" point to a side chain.
- "LMB-drag to sprout a new atom or bond" points to a terminal atom.
- "Hover mouse to change bond order: 1/2/3" points to a double bond.
- "LMB-click to change bond order: 1/2/3" points to another double bond.

A context menu is open over the molecule, titled "Bond RMB+click". The menu items are:

- Undo Optimize Alignment (Ctrl+Z)
- Redo Add Atom (Ctrl+Y)
- Select All (Ctrl+A)
- Invert Selection (Ctrl+I)
- Paste (Ctrl+V)
- Recenter View (Home)
- Delete (Del)
- Change Bond Order (highlighted)
 - Single 1
 - Double 2
 - Triple 3
- Save Image As...

The left sidebar contains an "Elements" panel with buttons for H, C, N, O, S, P, F, Cl, Br, I, B, Si, and rings for benzene, furan, pyrrole, and thiophene. Below it are "Select" options: Rotate Mode (unselected) and Select Mode (selected). A note says "Hold Ctrl" and "LM rotate, RM tra".

The top toolbar includes icons for Undo, Redo, Reset, Atoms, H, XEDs, Fields, Shape, Display, Color, Labels, Clear, Mol, +ve, -ve, vdW, Hyd, and Help. A version number "2.0" is also visible.

The right sidebar contains an "Information" panel with fields for Title ("New design") and Notes ("New design DPPIV"). Below it is a "Radial Plot" showing a hexagonal plot with axes labeled MW, Sim, SlogP, TPSA, and xibility. The plot has a green shaded area. The "Actions" panel at the bottom right includes buttons for Add H, Del H, Charge for pH7, Add Fields, Minimize, Optimize Alignment, Save a Copy, OK, Align, and Cancel.

At the bottom of the window, a status bar shows: "Median(pIC50) [Pred 6.7; Dist to model Excellent]" and "w/RM moves coordinates. Drag on an atom to draw."

L/RMB	Left/Right mouse button	Shortcut	Action
		Ctrl+A	Select all molecule
		Ctrl+I	Invert selection
		Shift+RMB-drag on any atom of selection	Translate a selection of the molecule