

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

Elements

H C
N O
S P
F Cl
Br I
B Si
- 0 +
[Ring icons]

Lines L
Thin Stick T
Capped Stick A
Ball and Stick Ctrl+L
CPK K

Index Shift+I
Element Shift+E
Type Shift+Y
Charge Shift+G
Formal Charge Ctrl+Shift+C
Field Size Shift+F
Chirality Shift+H
Residue Shift+R
Temperature Shift+T
Name Shift+N
Reset Labels Shift+X

Atom RMB+click

Undo Neutralise Atom(s) 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 Shift+C
Bromine B
Iodine I

Make Positive +
Make Neutral 0
Make Negative -

Information

Title: new design
 Keep source properties

Notes: new design DPP4

Radial Plot

0.686
Pred [02 Field for ...
MW Sim
Flexibility SlogP
TPSA

Actions

Add H Del H
Charge for pH7 Add Fields
Minimize
Optimize Alignment
Save a Copy
OK Align Cancel

Select
● Rotate Mode Rotate Mode
○ Select Mode

Score: 0.854 | 02 Field for Median(pIC50) [Pred 6.8; Dist to model Excellent]

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

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

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	Ctrl+RMB-drag	Z-clip the display

Information

Title: new design

Keep source properties

Notes: new design DPP4

Radial Plot

0.686

Pred (O2 Field for ...)

MW Sim

Flexibility SlogP

TPSA

Actions

Add H Del H

Charge for pH7 Add Fields

Minimize

Optimize Alignment

Save a Copy

OK Align Cancel

Hold Ctrl

an(pIC50) [Pred 6.8; Dist to model Excellent]

LM rotate, RM translate, MM scales. Shift-LM/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