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Ligand sketching and ligand importing to Biovia Discovery Studio



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Ligand:-

Ligand or guest or key. The complementary partner molecule which binds to the receptor. **Ligands** are most often small molecules but could also be another biopolymer. **Docking**. Computational simulation of a candidate **ligand** binding to a receptor.

Ligand sketching in Biovia Discovery Studio:-

- Open Discovery Studio Visualizer. In the Welcome windows click on Small molecule library under Small Molecules menu.
- This is the default visualization: molecule is represented as “Stick” corresponding to bonds; the bond order is shown (double bond are represented by two parallel sticks), the atoms are colored according to their type: carbon are grey, oxygen red, nitrogen blue, sulfur yellow, phosphorous violet and so on; hydrogens are not shown.



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➤ We can save the molecule in different supported formats like

Discovery Studio Files

Viewer Files

MDL MOL/SD Files

Sybyl MOL2 Files

Protein Data Bank Files

Comma Separated Files

Catalyst Files

Catalyst Query Files

Quanta Brick Map Files

SMILES Files

XYZ Coordinate Files



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CNX Map Files

POV-Ray Scene Files

VRML World Files

CHARMm Simulation Files

Image Files

DS ActiveX Control Files

Graphics Files



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Steps of Ligand sketching in Biovia Discovery Studio

1. First start the Discovery Studio by clicking on the icon on the desktop. Close the DS Welcome window by clicking on the small red close button.

2. Then open a new molecular window in Discovery Studio Visualizer,

Click on File

↓
New
↓

Molecular Window

3. After the sketch tool on, left click on the black colour structure visualization window to create a carbon atom and drag the mouse in any direction in which you need to grow the carbon chain.

4. Right Click on the Black colour Structure visualization window and the left click on Sketch button to start sketching a small molecular Structure.



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5. Left-Click again on the structure window to create another carbon connected with the previous with a single bond.
6. Continue left-clicking on the black color structure window to grow the carbon chain in the desired direction, either to make an open chain or can be taken back to the first atom to close the chain.
7. Alternatively carbon chains can be drawn by left clicking and dragging the mouse in desired direction while press holding the left mouse button.
8. To make a Ring carbon skeleton, right click on black color structure window and select Sketch ring tool.
9. Right Click on the Black color structure window and select Sketch ring tool to draw ring structures. While press holding the left mouse button on the structure window roll the middle mouse button, or drag finger over the touchpad to increase or decrease the ring size and then release the mouse button after getting a desired ring size.



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10. To make a branching on any carbon skeleton click on any carbon atom on the chain and go on dragging the mouse while press holding the left mouse button to get a desired branch length.

11. To change the Bond type use the sketch tool from right click on structure window and single click on any bond, not atoms, it will change to double bond, click once again to make it triple bond and once more to again make it a single bond back.