




Generating 3D structures in Avogadro:

- 1) Draw your desired compound in ChemDraw using as much perspective and stereochemical indicators as possible (draw in ring fusion hydrogens explicitly).
- 2) Save as a .mol file.
- 3) Open that .mol file in Avogadro and confirm that you want it to attempt to develop a 3D model.
- 4) Select the energy minimization tool  then click start and wait until the structure becomes mostly static then click stop.
- 5) Select the rotate tool  and look for any atoms that look distorted as this is usually an indication that the program selected the wrong stereochemistry for that atom.
- 6) Select the select atom tool  and select the atom in question. Invert the stereochemistry at that position by going to Build -> Invert Chirality in the menu.
- 7) Repeat 4-6 until the structure is correct.
- 8) Hit ctrl+s to save.
- 9) Upload the .mol file to the MaxBridge website and click submit job.

Generating 3D structures in Spartan:

- 1) Draw your desired compound in ChemDraw using as much perspective and stereochemical indicators as possible (draw in ring fusion hydrogens explicitly).
- 2) Save as a .mol file.
- 3) Open that .mol file in Spartan and confirm that you want it to convert to 3D.
- 4) Open the Build tool and minimize the structure
- 5) Find any atoms with improper stereochemistry and ctrl + double click to invert the stereochemistry.
- 6) Minimize the structure again.
- 7) Repeat 5 and 6 until the structure is correct.
- 8) Hit ctrl+s to save.
- 9) Upload the .mol file to the MaxBridge website and click submit job.

Generating 3D structures in Chem3D

- 1) Draw your desired compound in ChemDraw using as much perspective and stereochemical indicators as possible (draw in ring fusion hydrogens explicitly).


2) Save as a .mol file.

3) Open that .mol file in Chem3D.

4) Minimize the structure using the MM2 minimization button



5) Select the rotate tool  and look for any atoms with the wrong stereochemistry.

6) Select the select atom tool  and select the atom in question. Invert the stereochemistry at that position by going to Structure -> Invert in the menu.

7) Repeat 4-6 until the structure is correct.

8) Hit ctrl+s to save.

9) Upload the .mol file to the MaxBridge website and click submit job.