1. Ligand Building

Ligand is preferentially built with the Maestro software from Schrodinger suite. Avogadro can also be used. If The ligand is a known compound derivative, it is better to download it *(mol2 of pdb format)* from the pdb / pubchem / zinc databases to prevent construction mistakes.

Add atoms and chemical groups (to the initial compound in case of derivatives) until the desired structure is achieved. Special care must be taken to corretly assign the covalent bond types and groups charges. All the hydrogen atoms have to be build.

Finally, quickly optiomize the structure geometry (Ctrl+M in Maestro, Ctrl+Alt+O in Avogadro) and save the compound as a mol2 file.

1. Restraints calculation

Connect to Grade Web Server (http://grade.globalphasing.org/cgi-bin/grade/server.cgi).

Tick the box “Run grade on mol2 file” and upload your mol2 file.

Assign a three letter code and a name to your ligand and enter its overall charge.

Run grade