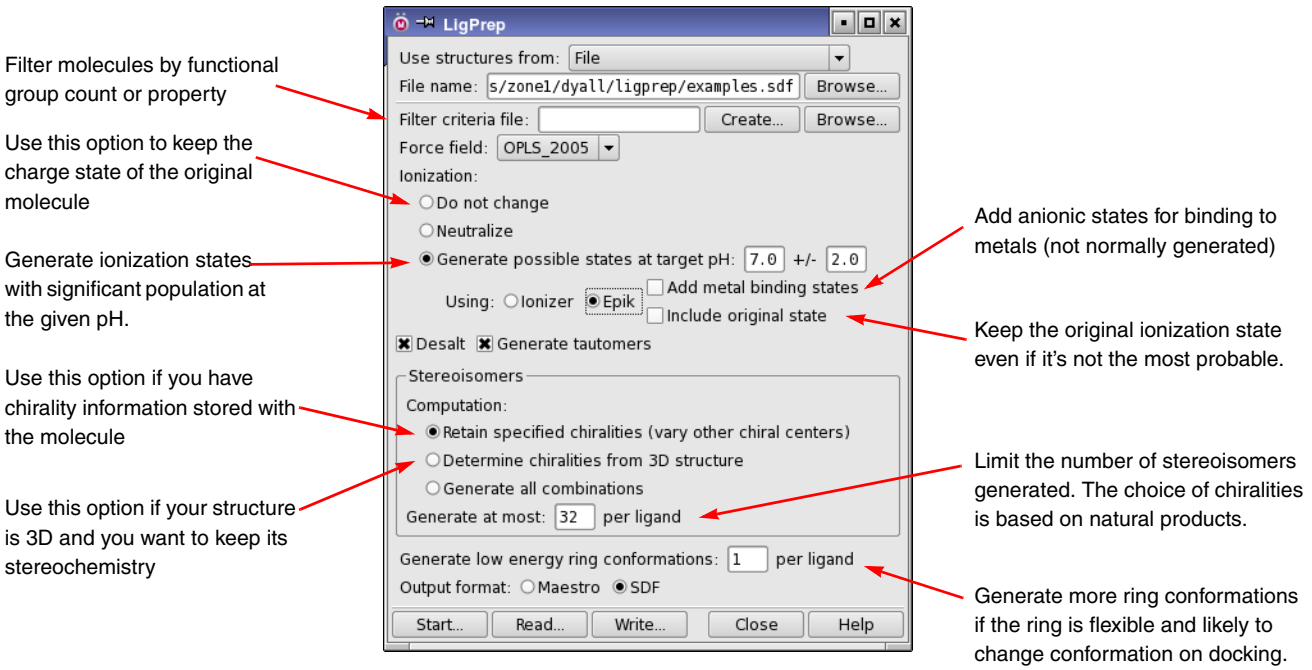
# Ligand Preparation

Proper preparation of 3D, all-atom ligand structures is critical to modeling tasks. The preparation involves the following tasks:

1. Add hydrogen atoms.
2. Filter out unsuitable molecules based on their properties.
3. Remove unwanted molecules, such as water, small ions.
4. Neutralize charged groups, then generate ionization and tautomeric states with Epik
5. Generate stereoisomers, particularly if stereochemical information is missing.
6. Generate low-energy ring conformations.
7. Remove any badly prepared structures.
8. Optimize the geometries.

This sheet summarizes ligand preparation with LigPrep.




1. Choose the source of the structures from the Use structures from option menu, and supply the file name if using a file.
2. Filter the structures by property by functional group counts—click Create to set up the filter.
3. Choose the force field. You usually only need to do this if the default doesn't cover some atom types in your ligands.
4. Choose an ionization option. Use of Epik is recommended.
5. Leave Desalt selected, to remove molecules other than the ligand.
6. Deselect Generate tautomers if you don't want to generate tautomers, for example to prepare just the original structures.
7. Choose an option for generating stereoisomers.
8. Increase the number of ring conformations if you have flexible rings that are likely to change conformation.
9. Select an output file format, and start the job.