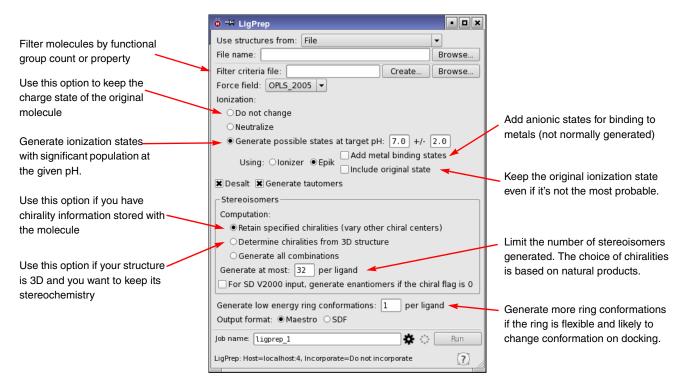
Ligand Preparation

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.