

# LigPrep

The screenshot shows the LigPrep application window. At the top, there are four navigation tabs: 'Prepare protein', 'Generate grid', 'Prepare ligands' (which is active and highlighted in blue), and 'Docking'. The main window contains several sections for configuring the ligand preparation process. Callouts with blue lines point to specific settings: 'Use structures from: File' (with a dropdown arrow), 'File name:' (with a 'Browse...' button), 'Filter criteria file:' (with 'Create...' and 'Browse...' buttons), 'Force field: OPLS3e' (with a 'Customize...' button and a 'Use customized version' checkbox), 'Ionization:' (with radio buttons for 'Do not change', 'Neutralize', and 'Generate possible states at target pH: 7.0 +/- 2.0'), 'Using: Ionizer' (radio button) and 'Epik' (radio button, which is selected), 'Add metal binding states' (checkbox), 'Include original state' (checkbox), 'Desalt' (checked checkbox) and 'Generate tautomers' (checked checkbox), 'Stereoisomers' section with 'Computation:' (radio buttons for 'Retain specified chiralities (vary other chiral centers)', 'Determine chiralities from 3D structure', and 'Generate all combinations'), 'Generate at most: 32 per ligand' (text box), 'For SD V2000 input, generate enantiomers if the chiral flag is 0' (checkbox), 'Output format: Maestro' (radio button, selected) and 'SDF' (radio button), 'Job name: ligprep\_example' (text box), and a 'Run' button. The status bar at the bottom shows 'Host=localhost:4, Incorporate=Append new entries as a new group' and a help icon.

Use structures from: File

File name: Browse...

Filter criteria file: Create... Browse...

Force field: OPLS3e Customize... Use customized version

Ionization:

☐ Do not change

☐ Neutralize

☒ Generate possible states at target pH: 7.0 +/- 2.0

Using: ☐ Ionizer ☒ Epik ☐ Add metal binding states ☐ Include original state

☒ Desalt ☒ Generate tautomers

Stereoisomers

Computation:

☒ Retain specified chiralities (vary other chiral centers)

☐ Determine chiralities from 3D structure

☐ Generate all combinations

Generate at most: 32 per ligand

☐ For SD V2000 input, generate enantiomers if the chiral flag is 0

Output format: ☒ Maestro ☐ SDF

Job name: ligprep\_example Run

Host=localhost:4, Incorporate=Append new entries as a new group ?

Acceptable inputs include Workspace, Project Table and File (.mae, .smi, .mol, .sdf, and .csv, are among the accepted file types)

The forcefield is used for the minimization of structures during the preparation process

For more information on Epik, go to [schrodinger.com/epik](http://schrodinger.com/epik)

Make sure that pH set for generating ionization states agrees with the pH of the system being considered

## Retain specified chirality

Keep the information on chiralities from the input file, and fix these chiralities for the entire calculation.

## Determine chiralities from 3D structure

Discard all chirality information in the input file, and determine the chirality from the 3D geometry. These chiralities are held fixed. For centers whose chirality is indeterminate, structures for the two possible chiralities for each center are generated.

## Generate all combinations

Discard all chirality information, both from input file properties and from the 3D geometry, and generate all possible configurations that result from the combination of chiralities on each chiral center.

Specify the file format for the output file. If you want to incorporate the structures into the current project, you must select Maestro for the format. In SDF format, the structures are written to the file `jobname.sdf`.