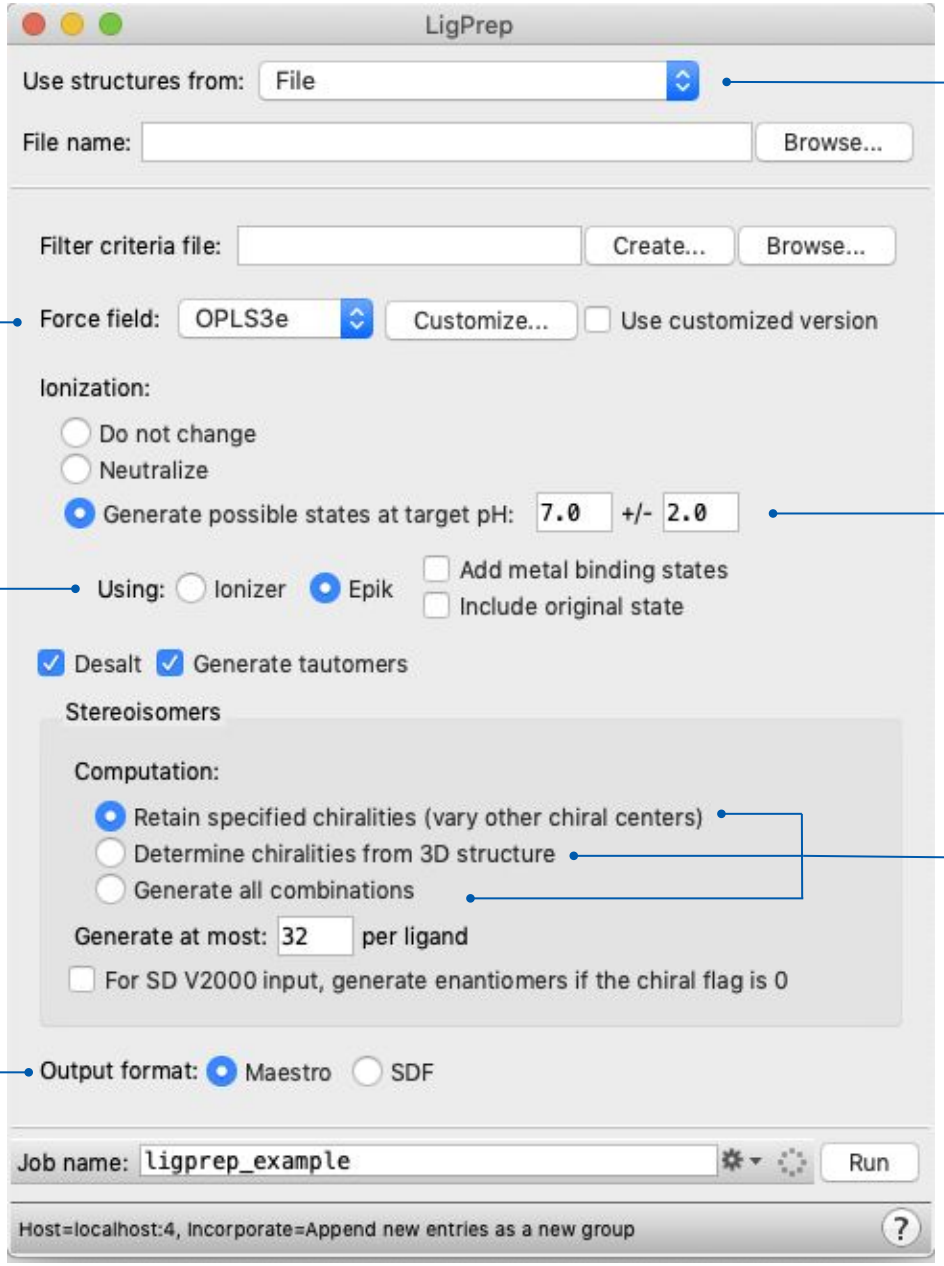
LigPrep



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

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

For more information on Epik, go to schrodinger.com/epik

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.