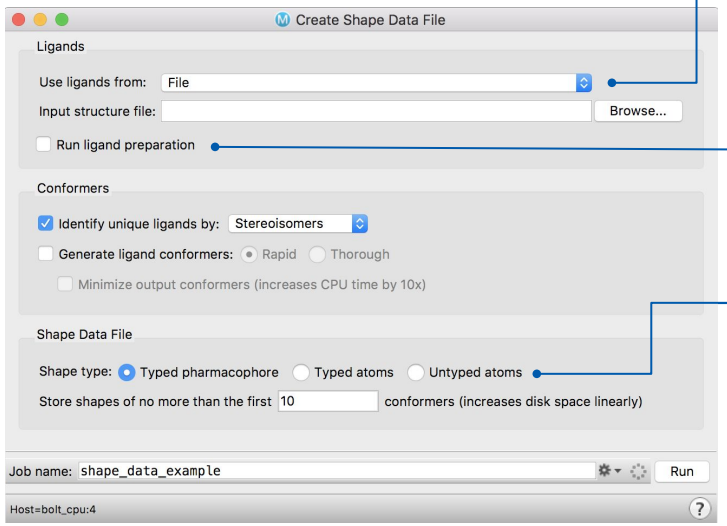
GPU Shape

1. Create Shape Data File

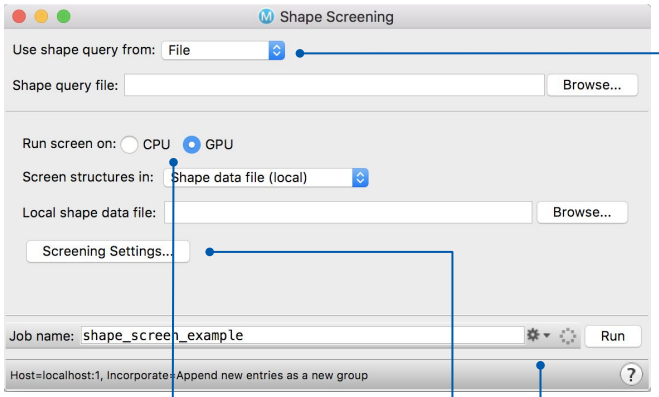


Acceptable inputs include Selected Entries, File and both local and remote Phase Databases

Only necessary when input structures have not gone through LigPrep

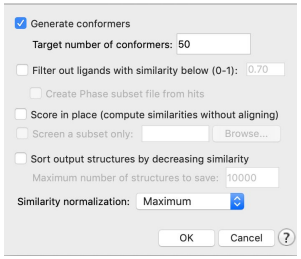
Validation testing suggests using unminimized conformers with a Typed pharmacophore shape type to maximize enrichment

2. Shape Screening



Validation testing suggests using ~10 query structures as probes in the GPU Shape Screen for best enrichment (Note: screen time scales with the number of probes used)

Click on the Gear icon and make sure to switch to a GPU host



*There is a **~50x** speedup when running Shape on GPU compared to CPU*