

# 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

Use ligands from: File

Input structure file: Browse...

Run ligand preparation

Conformers

Identify unique ligands by: Stereoisomers

Generate ligand conformers: Rapid Thorough

Minimize output conformers (increases CPU time by 10x)

Shape Data File

Shape type: Typed pharmacophore Typed atoms Untyped atoms

Store shapes of no more than the first 10 conformers (increases disk space linearly)

Job name: shape\_data\_example

Host: bolt\_cpu:4

Use shape query from: File

Shape query file: Browse...

Run screen on: CPU GPU

Screen structures in: Shape data file (local)

Local shape data file: Browse...

Screening Settings...

Job name: shape\_screen\_example

Host: localhost:1, Incorporate+Append new entries as a new group

Generate conformers

Target number of conformers: 50

Filter out ligands with similarity below (0-1): 0.70

Create Phase subset file from hits

Score in place (compute similarities without aligning)

Screen a subset only: Browse...

Sort output structures by decreasing similarity

Maximum number of structures to save: 10000

Similarity normalization: Maximum

OK Cancel