

Launching DROIDS v2.0

1. Open Linux terminal from downloaded DROIDS folder and type 'perl DROIDS.pl' to open GUI
2. Identify paths for paths.ctl file (first time only ..else skip)
3. Choose Type of Analysis, No. of GPU, Amber16/18

DROIDS Amber/cpptraj/parsing GUI

1. specify query and reference PDB files in your DROIDS folder
2. Specify number of production run samples to take (note: 50-100)
3. Check box for solvation method (note: explicit takes longer and uses considerably more memory)
4. Specify the length of heating, equilibration, and each production run (note: energy minimization step is hard coded)
5. Create MD and DROIDS control files
6. Click on the alignment button and USCF Chimera will open and you will be prompted at terminal to use MatchMaker and Match->Align to create a Clustal (.aln) file as well as to choose the residue from which you want to reference your atom correlations. Simply close Chimera to continue on.
7. Create/check your topology and coordinate files using teLeap button. Read the terminal output carefully here.
8. Launch MD runs (note: MD runs can be monitored at the main Linux and GPU surveillance terminals. The cpptraj buttons follow ccpraj control files, atom info files, atom fluctuation files.
9. Click 'prepare/parse files for DROIDS' and follow directions on main Linux terminal.
10. DROIDS STATS GUI will open when final parsing is done.

DROIDS statistical analysis GUI

1. Enter significance level for hypothesis testing and method for multiple test corrections
2. Run statistical tests (note: R graphics plots and data files will appear in resulting folder for each analysis)

DROIDS image analysis GUI

1. Enter number of frames for movies.
2. Choose visualization options for Chimera protein representation, types of motion to analyze, type of K-S test result to view, corresponding color scheme, and method of multiple test correction.
3. Create chimera attribute file and display these results on static PDB structure in the Chimera viewer
4. Render movies on XYZ axes of the reference PDB and display in DROIDS movie viewer