

Prepare

gau_prmtop2gaucom.py (former amboniom.py)

Convert Amber topology to ONIOM model.

gau_freezecom.py (former gfreezer.py)

Freeze complete residues beyond specified distance.

gau_setscan.py (former gscan.py)

Specify target distance (or number of steps) of a scan.

Analysis

gau_makepdb.py (former g2pdb.py)

Make a .pdb file from .log or .com.

gau_plot2dscan.py (former gsurf.py)

Plot energy as a function of 2 coordinates in 3D space.

gau_checklog.py (former hiig.py)

Check energies and convergence status.

gau_energies.py (former g09out_analysis.py)

Print energies to .csv file for analysis in spreadsheet.

gau_measure.py

Measure distance, angle or dihedral.

Restart

gau_autorestart.py (former paimei.py)

Automatically restart calculations on linux cluster. Specially useful for microiterations and internal coordinates errors.

gau_log2com.py (former gx.py)

Make a new .com file from any opt/scan point from a .log file.

Miscellaneous

gau_add_line.py

Resolve Gaussview problem in reading all .log lines as ModRed.