Docs for qt_scripts

1 Table-like

For full description of usage run the scripts with `--help` or `-h`

1.1 prepare ONIOM inputs

	In	Out	Motivation
`amboniom.py`	`.prmtop` (or `.top`) plus `.inpcrd` (or `.crd` / `.rst`)	`.com`	Exact copy of forcefield parameters from Amber topology to gaussian.com file. Specially useful with parameterized ligands and newer forcefields (gaussian uses ff94 by default).
`gfreezer.py`	`.com`	`.com`	Freeze protein further than a distance from high layer. Can be used to generate an external layer of water molecules.

1.2 monitor and analysis

	In	Out	Motivation
`g2pdb.py`	`.log` / `.com`	`.pdb`	Visualize scans and optimizations in VMD or Pymol by producing a .pdb file.
`hiig.py`	`.log`		Get convergence situation of a job and a plot of energy along scan or optimization.
`gsurf.py`	any number of `.log` files	3D plot	Plot energy against 2 reaction coordinates in a 3D plot.

1.3 restart jobs

	In	Out	Motivation
`gx.py`	`.log`	`.com`	Restart calculation from a specific scan point (the last by default).
`gscan.py`	`.com`	`.com`	Automatically set up scans by specifing final distance of reaction coordinate.
`paimei.py`			Automatically restarts error jobs. Works well with scans and ground state optimizations. Read the manual for instructions.

2 Standardization of options

This is yet to be implemented, if we all agree.

- `-o` — optimization steps
- `-s` — scan steps
- `--out` — filename for output of script
- `-e` — energy type (oniom/scf/low)