**Version Information 10/21**

This is the 1st released version.

Comment out “setting PYTHON environment” in MGLTools prepare\_ligand4.py to avoid this in output screen.

The next version will contain, not in any order:

* Penalties and constraints are implemented easily and should also be made for the specific molecule and goal. Examples of hydrogen bond requirements and sub-structure restrictions is to be included.
* Specificity in choosing random heavy atoms or points such as bonds in some of the molecular modifications to be included. This will give a slight increase in computational performance.
* OPEN\_BOND in ring opening is to be included.
* Multiple proteins and sites to be included for screening against toxicity and penalizing unwanted binding.
* The software is designed to include database information. The octanol-water partition coefficient is to be included in the orally ingested ADME restriction by accessing database information. Substructure constraints using known pieces of known molecules to be included.
* Pseudo-atom included with naming X0001 etc… This requires fixed format changes of the SMILES expressions and translation to SMILES in the functions.
* Ring limit of 9 removed.
* Create more parallel mutation and crossover operations in GA. This is not the docking with GOLD, which is in parallel and the most computationally consuming part of Ligand GA for non-simple molecules. The improvement is in the mutation/crossover functions. In progress.
* Output during run is commented out. Uncomment output as an option.
* Including solvent and a more precise measure of docking using protein\_ligand in solvent minus protein in solvent minus ligand in solvent.
* Possible removal of MGLTools in exchange for Matlab code.
* …
* GUI

Suggestions for changes or additions are welcome.