

To run examples:

1. Run all examples in this directory.
 - a. "python runAllExamples.py"
 - b. output files from input files in inSmi/ will be *_fromSmiles.cif and *_fromSmiles.pdb
 - c. output files from input files in inMol/ will be *_fromMol.cif and *_fromMol.pdb
 - d. output files from input files in inMmcif/ will be *_fromMmcif.cif and *_fromMmcif.pdb
2. Run an individual example input file.
 - a. Run an input file from a SMILES file at inSmi/.
 - i. E.g. "acedrg -i inSmi/DB00201.smiles -o DB00201
 - ii. The output files are DB00201.cif (the dictionary file) and DB00201.pdb (the coordinate file)
 - b. Run an input file from a Mol file at inMol/.
 - i. E.g. "acedrg -m inMol/DB00201.mol -o DB00201
 - ii. The output files are DB00201.cif (the dictionary file) and DB00201.pdb (the coordinate file)
 - c. Run an input file from a mmCIF file at inMmcif/.
 - i. E.g. "acedrg -c inMmcif/DB00201.cif -o DB00201
 - ii. The output files are DB00201.cif (the dictionary file) and DB00201.pdb (the coordinate file)